

Exposure Profiles for HAPs -- Group 1

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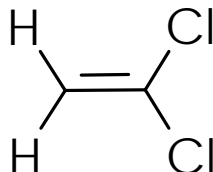
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VINYLDENE CHLORIDE

SUBSTANCE IDENTIFICATION

Synonyms: 1,1-Dichloroethylene; 1,1-dichloroethene; 1,1-DCE; VDC

Structure:



CAS Registry Number: 75-35-4

Molecular Formula: C₂H₂Cl₂

CHEMICAL AND PHYSICAL PROPERTIES

Boiling Point: 31.7 °C

Melting Point: -122.5 °C

Molecular Weight: 96.95

Dissociation Constants:

Log Octanol/Water Partition Coefficient (log K_{ow}): 2.13 (1)

Water Solubility: 2250 mg/L @ 25 °C (2)

Vapor Pressure: 498 mm Hg @ 20 °C (5); 600 mm Hg @ 25 °C (3)

Henry's Law Constant: 2.61 x 10⁻² atm-m³/mole @ 24 °C (4)

Lower Explosive Limit: 5.6% @ 25 °C (5)

[(1) Hansch C, Leo AJ; Medchem Project Issue No 26 Claremont, CA: Pomona College (1985) (2) Delassus PT, Schmidt DD; J Chem Eng Data 26: 274-6 (1981) (3) Boublik T et al; The Vapor Pressures of Pure Substances. p. 96. Amsterdam: Elsevier (1984) (4) Gossett RW; Environ Sci Technol 21: 202-206 (1987) (5) Dreher E-L; Ullmann's Encyclopedia of Industrial Chemistry, 5th ed A6: 294-297 (1986) (5) ITI; Tox and Haz Indus Chemical Safety Manual p. 555 (1982)]

EXPOSURE PROFILE

Production: No current non-CBI production data were available for vinylidene chloride. U.S. demand for vinylidene chloride was 68,000 metric tons (150 million pounds) in 1987 and was projected to rise to 79,000 metric tons (170 million pounds) in 1992 (4). Estimated 1989 production of vinylidene chloride was 230 million pounds (5). Vinylidene chloride is produced by Dow Chemical U.S.A. (Freeport, TX) and PPG Industries, Inc. (Lake Charles, LA) (1, 2). Vinylidene chloride is almost exclusively produced from 1,1,2-trichloroethane, primarily by liquid-phase dechlorination in the presence of alkali (3).

[(1) USITC; Synthetic Organic Chemicals. United States Production and Sales, 1991. USITC Publication 2607. pp. 15-33. February 1993 (2) SRI International; 1993 Directory of Chemical Producers, United States of America. p. 1006 (1993) (3) Dreher E-L; Ullmann's Encyclopedia of Industrial Chemistry, 5th ed. A6: 294-297 (1986) (4) Reed DJ; Kirk-Othmer Encyclopedia of Chemical Technology, 4th ed. 5: 1017-1028 (1993) (5) Chemical Manufacturer's Association (CMA); Written communication: Public comment on Toxicological Profile for 1,1-Dichloroethene. Washington, DC, May 12, 1989)]

Use: Vinylidene chloride is used to manufacture poly(vinylidene chloride) (PVDC) and its copolymers with vinyl chloride, acrylonitrile, and acrylates (1, 2). These polymers have outstanding resistance to chemical attack and are efficient gas barriers. They are used for food packaging films (e.g., Saran wrap), in paints and coatings, and coatings in controlled-release fertilizers (1-4). Vinylidene chloride can also be used captively for the production of 1,1,1-trichloroethane; however, this method of manufacturing 1,1,1-trichloroethane was largely replaced in the late 1970s (1, 5). Approximately 60-80% of vinylidene chloride production is used to manufacture PVDC and its copolymers; the rest is converted into 1,1,1-trichloroethane (1).

[(1) Dreher E-L; Ullmann's Encyclopedia of Industrial Chemistry, 5th ed. A6: 294-297 (1986) (2) Heiling P; Ullmann's Encyclopedia of Industrial Chemistry, 5th ed. A18: 380 (1991) (3) Goertz HM; Kirk-Othmer Encyclopedia of Chemical Technology, 4th ed. 7: 270 (1993) (4) Wicks ZW Jr; Kirk-Othmer Encyclopedia of Chemical Technology, 4th ed. 6: 737 (1993) (5) U.S. EPA; Locating and estimating air emissions from sources of vinylidene chloride. EPA-450-4-84-007k. EPA, Office of Air Quality Planning and Standards, Research Triangle Park, NC (1985)]

Occupational Exposure: NIOSH (NOES Survey 1981-83) has statistically estimated that 2,675 workers are exposed to vinylidene chloride in the United States (1). Vinylidene chloride concentrations in monomer and polymer manufacturing plants have been reported to be 90-100 $\mu\text{g}/\text{m}^3$ (22-25 ppb) and 25-50 $\mu\text{g}/\text{m}^3$ (6.2-12 ppb), respectively (3). Levels as high as 7,700 mg/m^3 (1,900 ppm) were found in a vinylidene chloride-ethyl acrylate copolymer monofilament fibre production plant (4). Estimated TWA exposure levels for different job categories in this plant ranged from 6 to 70 ppm (4). Worker exposure of $<20 \text{ mg}/\text{m}^3$ ($<5 \text{ ppm}$) and trace levels were reported for polymer manufacturing plants (5). Vinylidene chloride levels of 2.6-256 mg/m^3 (0.6-63 ppm) have been reported in telephone offices across the U.S. (5). Air in submarines and spacecraft contained 8 and 0-8 mg/m^3 (2 and 0-2 ppm), respectively (5).

Vinylidene chloride is produced by the thermal decomposition of 1,1,1-trichloroethane, a reaction that is catalyzed by copper (2). Since 1,1,1-trichloroethane is used as a degreasing agent in welding shops, there is a potential for vinylidene chloride to be formed in these shops as well as in other industrial environments where 1,1,1-trichloroethane is used near sources of heat.

[(1) NIOSH. National Institute for Occupational Safety and Health. National Occupational Exposure Survey (NOES). Computer printout March 29, 1989 (2) Glisson BT; Am Ind Hyg Assoc J 47: 427-435 (1986) (3) U.S. EPA; Health assessment document for vinylidene chloride. EPA-600/8-83-031F, Office of Health and Environmental Assessment, Washington, DC (1985) (4) Ott MG et al; J Occup Med 18: 735-8 (1976) (5) IARC; Monograph on the Evaluation of the Carcinogenic Risk of Chemicals to Humans Volume 39 pp. 195-226 (1986)]

Consumer Exposure: Vinylidene chloride is a known contaminant in plastic wrap made from this monomer (1). Residual vinylidene chloride has been detected in food packaging films ranging from <0.02 to 1.26 ppm; residues in a variety of foodstuffs wrapped in the film were \leq 0.005 to 0.01 ppm (2). Another investigator found residual vinylidene chloride of 6.5 to 10.4 ppm in food wrap (3).

[(1) Fishbein L; Sci Total Environ 11: 111-61 (1979) (2) Gilbert J et al; J Chromatography 197: 71-8 (1980) (3) Birkel TJ et al; J Assoc Off Anal Chem 60: 1210-3 (1977)]

Environmental Release and General Population Exposure: According to the 1991 Toxics Release Inventory (TRI), 286,037 pounds of vinylidene chloride were released to the environment, of which 99.7% was released into the atmosphere (1). The following industrial processes have been identified as potential sources of vinylidene chloride emissions: vinylidene chloride production, tetrachloroethylene and trichloroethylene production, 1,1,1-trichloroethane production, vinylidene chloride polymerization, use of vinylidene chloride in specialty chemical production, vinylidene chloride copolymer fabrication, and volatilization from waste treatment, storage, and disposal (14). Emission factors (grams of vinylidene chloride released per gram of product) and source locations have been estimated by EPA (14). Vinylidene chloride is a product of the hydrolysis of 1,1,1-trichloroethane (8). It is also formed biotically from trichloroethylene under anaerobic conditions, such as may be found in landfills and groundwater (9, 22, 24). A formation rate at 20 °C and neutral pH is 0.040 year⁻¹ (22). Therefore, vinylidene chloride may be formed by these processes in landfills or groundwater polluted with chlorinated solvents. Vinylidene chloride is also produced by the thermal decomposition of 1,1,1-trichloroethane, a commonly used solvent, and may therefore be emitted from incinerators burning waste solvents (10). Vinylidene chloride was emitted from an incinerator burning waste plastics and solvent at 388-653 mg/hour (7).

A correlation of data from the EPA Air Toxics Emission Inventory with industrial source categories (SIC codes), shows that emissions of vinylidene chloride are associated with coated fabrics and finishing plants, plastic materials and resins, synthetic rubber and fibers, pharmaceuticals, paints, industrial organic chemicals, electrical lighting and wiring equipment, surgical supplies, photographic equipment and supplies, and sanitary services (11).

In a comprehensive survey of wastewater from 4,000 industrial and publicly owned treatment works (POTWs) sponsored by the Effluent Guidelines Division of the U.S. EPA, vinylidene chloride was identified in discharges of the following industrial categories (frequency of occurrence; median concentration in ppb): timber products (2; 10.8), steam electric (2; 38.8), petroleum refining (1; 8.0), nonferrous metals (3; 2.9), paint and ink (1; 4.6), printing and publishing (1; 152.6), organics and plastics (31; 35.7), inorganic chemicals (2; 20.7), pulp and paper (4; 9.3), rubber processing (1; 137.7), auto and other laundries (6; 32.8), pesticides manufacture (2; 246.8), organic chemicals (2; 675.8), transportation equipment (1; 238.0), and POTWs (40; 23.0) (2). The highest effluent concentration was 3,636 ppb in the auto and other laundries industry (2).

The median, 75th percentile, and maximum concentrations of vinylidene chloride in urban and suburban areas of the U.S. (325 samples) were 0.0050, 0.0075, and 0.14 ppb, respectively (3). In two rural areas, the vinylidene chloride concentrations were <0.005 ppb (Pullman, WA) (4) and 0.065 ppb (Grand Canyon, AZ) (5). The median and maximum concentrations in source-dominated areas were 3.6 and 6.7 ppb, respectively (3). In two cities where vinylidene chloride was manufactured, the mean concentrations were 0.13 ppb (Freeport, TX, 1 sample) and 6.7 ppb (Lake Charles, LA, 5 samples) (3). The geometric mean concentration of vinylidene chloride in three New Jersey Cities, Newark, Elizabeth, and Camden, in 1981/1982 ranged from 0.35 to 0.38 ppb in the summer with 95% of samples positive and 0.31 to 1.02 ppb in the winter with 85% of samples positive (12). Vinylidene chloride was found in 4 of 15 samples of indoor air taken during the summer at 1.8-93.6 ppb and 4 of 16 samples taken during the winter at 5.0-9.6 ppb (6). None of the chemical was found in parallel samples taken out-of-doors (6). No correlation was found between the presence of vinylidene chloride in indoor air and structural characteristics of the dwelling or activity (6).

In EPA's Groundwater Supply Survey, 24 of the 945 finished water supplies that use groundwater sources contained vinylidene chloride up to 6.3 ppb (15). Of 13 U.S. cities surveyed that obtained drinking water from groundwater sources, only one contained vinylidene chloride (0.2 ppb), whereas two of the 103 cities obtaining water from surface water contained vinylidene chloride (0.2 and 0.51 ppb) (16). Raw water serving two of the ground water supplies contained vinylidene chloride, whereas none of the raw surface water contained the chemical (16). In a screening of 1,174 community wells and 617 private wells in Wisconsin, 1 community and 3 private wells had detectable levels of vinylidene chloride (17). Two New Jersey supplies serving roughly 100,000 persons each contained mean and maximum concentrations of vinylidene chloride ranging from 0.1-0.2 and 0.9-2.5 ppb, respectively (18). Contaminated drinking water wells in New Jersey, Massachusetts, and Maine had maximum vinylidene chloride concentrations of 280, 118, and 70 ppb, respectively (19). Vinylidene chloride was detected in groundwater at 25.2% of 178 CERCLA sites (23). It was detected in groundwater samples from 9.5% of the 2,793 hazardous waste sites participating in EPA's Contract Laboratory Program; the geometric mean concentration was 1.38 mg/L (20).

Of the 4,972 surface water samples from three tributaries of the Ohio River and 7 of 8 sites on the Ohio River mainstream, 6.9% contained vinylidene chloride; 304 samples contained levels from 0.1 to 1.0 ppb, 36 samples from 1.0 to 10 ppb, and 3 samples >10 ppb (21).

Twelve percent of approximately 300 breath samples from Elizabeth and Bayonne, New Jersey contained quantifiable levels ($>0.2\text{-}2\text{ }\mu\text{g}/\text{m}^3$) of vinylidene chloride (13).

[(1) U.S. EPA; Toxics Release Inventory (1992) (2) Shackelford W; *Analyt Chim Acta* 146: 15-27 (supplementary data) (1983) (3) Brodzinsky R, Singh HB; *Volatile Organic Chemicals in the Atmosphere: An Assessment of Available Data* pp. 104-5. SRI International Contract 68-02-3452 (1982) (4) Grimsrud EP, Rasmussen RA; *Atmos Environ* 9: 1014-7 (1975) (5) Pellizzari ED; *Quantification of chlorinated hydrocarbons in previously collected air samples* EPA-450/3-78-112 (1978) (6) Pleil JD; *Volatile Organic compounds in indoor air: A survey of various structures* EPA-600/D-85-100 (1985) (7) Oki N et al; *Chemosphere* 21: 761-770 (1990) (8) Haag WR, Mill T; *Environ Sci Technol* 22: 658-663 (1988) (9) Hallen RT et al; *ACS Div Environ Chem 192nd Natl Mtg* 26: 344-6 (1986) (10) Glisson BT; Am

Ind Hyg Assoc J 47: 427-435 (1986) (11) Pacific Environmental Services; Toxic Air Pollutant/ Source Crosswalk - A screening tool for locating possible sources emitting toxic air pollutants. EPA-450/4-87-023a (1987) (12) Harkov R et al; Volatile organic compounds at urban sites in New Jersey. pp. 69-88 in Toxic Air Pollution. Chelsea, MI: Lewis Publ Inc (1987) (13) Wallace L et al; J Occu Med 28: 603-7 (1986) (14) U.S. EPA; Locating and estimating air emissions from sources of vinylidene chloride. EPA-450-4-84-007k. EPA, Office of Air Quality Planning and Standards, Research Triangle Park, NC (1985) (15) Westrick JJ et al; J Am Water Works Assoc 76: 52-9 (1984) (16) Coniglio WA et al; The occurrence of volatile organics in drinking water exposure assessment project. Criteria and Standards Division, Science and Technology Branch (1980) (17) Krill RM, Sonzogni WC; J Am Water Works Assoc 78: 70-5 (1986) (18) Wallace LA et al; Environ Res 43: 290-307 (1987) (19) Burmaster DE; Environ 24: 6-13,33-6 (1982) (20) U.S. EPA; Contract Laboratory Program Statistical Database. National Priorities Listing (1988) as cited in Agency for Toxic Substances and Disease Registry; Toxicological Profile for 1,1-Dichloroethene, p. 90. December, 1989 (21) Ohio River Valley Water Sanit Comm; Assessment of water quality conditions, Ohio River Mainstream 1980-81 Cincinnati, OH (1982) (22) Vogel TM, McCarty PL; J Contam Hydrology 1: 299-308 (1987) (23) Plumb RH; Groundwater Monit Review 7: 94-120 (1987) (24) Baek NH et al; J Environ Sci Health A25: 987-1005 (1990)]

Environmental Transport and Persistence:

Bioaccumulation: The log BCF for vinylidene chloride estimated from its log K_{ow} using a recommended regression equation is 25 (1). Therefore, vinylidene chloride would not be expected to bioconcentrate in fish.

[(1) Lyman WJ et al; Handbook of Chemical Property Estimation Methods New York, NY: McGraw-Hill p.5-5 (Eqn 5-2)]

Volatilization/ Adsorption: According to a simple fugacity model, vinylidene chloride will distribute almost entirely to air (99.87%); the remaining 0.13% will distribute to soil (3). Using the Henry's Law constant, the volatilization half-life for vinylidene chloride from a model river 1 m deep with a current of 1 m/s and a wind of 3 m/s is estimated to be 2.9 hours (1). Similarly, the volatilization half-life for a model lake 1 m deep with a 0.05 m/s current and 0.5 m/s wind is 3.9 days. An EPA pilot-scale study of VOC partitioning in conventional wastewater treatment showed that over 98% of vinylidene chloride entering the pilot plant volatilized (5). The soil adsorption coefficients, K_{oc} , for vinylidene chloride estimated from its water solubility using a recommended regression equation is 63 (1). A K_{oc} of 35 is predicted on the basis of molecular structure (4). These K_{oc} values suggest that vinylidene chloride would exhibit high to very high mobility in soil (2).

[(1) Lyman WJ et al; Handbook of Chemical Property Estimation Methods New York, NY: McGraw-Hill p. 4-9 to 4-10 (Eqn 4-5), 15-1 to 15-32 (1982) (2) Swann RL et al; Res Rev 85: 17-28 (1983) (3) U.S. EPA; PCGEMS (Graphical Exposure Modeling System), PCENPART (Environmental Partitioning Model) (4) Meylan WM et al; Environ Sci Technol 26: 1560-7 (1992) (5) U.S. EPA; Locating and estimating air emissions from sources of vinylidene chloride. EPA-450-4-84-007k. EPA, Office of Air Quality Planning and Standards, Research Triangle Park, NC (1985)]

Persistence: Vinylidene chloride reacts with photochemically-produced hydroxyl radicals in the atmosphere with a rate of 8.1×10^{-12} cm³/molecule-s (1). Assuming a hydroxyl radical concentration of 5×10^5 radicals/cm³, the half-life of vinylidene chloride in the atmosphere will be 2.0 days. Atmospheric reactions with ozone and NO₃ radicals will be

of minor importance in vinylidene chloride removal (2). The basic hydrolysis rate constant for vinylidene chloride at 25 °C is 1.09×10^{-7} L/mole-min and therefore, hydrolysis will be inconsequential (20,000 years at pH 9) (3).

Few studies are available on the aerobic biodegradation of vinylidene chloride. Generally, there is no evidence for aerobic biodegradation in chlorinated ethenes (5, 10, 11). One study presented contradictory results and reported that 30-54% of vinylidene chloride was removed after one week's incubation with a wastewater inoculum after correcting for volatilization losses (4). Under anaerobic conditions in microcosms designed to simulate the anaerobic conditions in groundwater and landfills, vinylidene chloride undergoes reductive dechlorination to vinyl chloride (6, 7, 8, 12). After 107 days in a batch fermenter, 56% of the vinylidene chloride was transformed to vinyl chloride and another 6% was mineralized (6). In microcosms designed to simulate a groundwater environment, 50% of the vinylidene chloride disappeared in 5-6 months (7). Under simulated landfill conditions, degradation occurred in 1-3 weeks (8). Approximately 50% of vinylidene chloride was converted to vinyl chloride by a mixed bacterial culture of carbon fermenters and methanogens in a month (9). After 40 weeks of incubation in three microcosms with methanogenic aquifer material, the vinylidene chloride concentration was reduced to <2, <2, and 39% of controls (12).

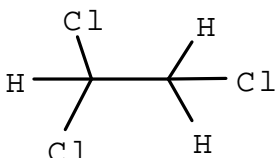
[(1) Atkinson R; J Phys Chem Ref Data. Monograph 1 (1989) (2) Grosjean D; J Air Waste Manage Assoc 41: 182-189 (1991) (3) Jeffers PM et al; Environ Sci Technol 23: 965-9 (1989) (4) Tabak HH et al; J Water Pollut Control Fed 53: 1503-18 (1981) (5) Bouwer EJ et al; Environ Sci Technol 15: 596-9 (1981) (6) Vogel TM, McCarty PL; Environ Sci Technol 21: 1208-13 (1987) (7) Barrio-Lage G et al; Environ Sci Technol 20: 96-9 (1986) (8) Hallen RT et al; Am Chem Soc Div Environ Chem 26th Natl Mtg pp. 344-6 (1986) (9) Baek NH et al; J Environ Sci Health A25: 987-1005 (1990) (10) McCarty PL, Roberts PV; Am Chem Soc Div Environ Chem 27th Natl Mtg pp. 129-32 (1987) (11) Pearson CR, McConnell G; Proc R Soc London B 189: 305-332 (1975) (12) Wilson BH et al; Environ Sci Technol 20: 997-1002 (1986)]

1,1,2-TRICHLOROETHANE

SUBSTANCE IDENTIFICATION

Synonyms: There are no commonly used synonyms.

Structure:



CAS Registry Number: 79-00-5

Molecular Formula: $C_2H_3Cl_3$

CHEMICAL AND PHYSICAL PROPERTIES

Boiling Point: 113.8 °C

Melting Point: -36.5 °C

Molecular Weight: 133.40

Dissociation Constants:

Log Octanol/Water Partition Coefficient (log K_{ow}): 2.07 (estimated, 1)

Water Solubility: 4420 mg/L @ 25 °C (2)

Vapor Pressure: 23.05 mm Hg @ 25 °C (3)

Henry's Law Constant: 8.24×10^{-4} atm-m³/mole @ 25 °C (4)

Lower Explosive Limit: 6% @ 25 °C (5)

[(1) Hansch C, Leo AJ; Medchem Project Issue No 26 Claremont, CA: Pomona College (1985) (2) Dilling WL; Environ Sci Technol 11: 405-9 (1977) (3) Daubert TE, Danner RP; Data Compilation Tables of Properties of Pure Compounds New York, NY: Amer Inst for Phys Prop Data (1989) (4) Leighton DT Jr, Calo JM; J Chem Eng 26: 382-5 (1981) (5) NIOSH; NIOSH Pocket Guide Chem Haz, 5th prt. p. 228 (1985)]

EXPOSURE PROFILE

Production: No non-CBI production information was available for 1,1,2-trichloroethane. Since the primary use of 1,1,2-trichloroethane is to produce vinylidene chloride and vinylidene chloride is produced almost exclusively from 1,1,2-trichloroethane (3), demand for 1,1,2-trichloroethane can be estimated from vinylidene chloride production. Since the U.S. demand for vinylidene chloride was 68,000 metric tons in 1987 and was projected to rise to 79,000 metric tons in 1992 (4), the corresponding 1987 demand and 1992 projected demand for 1,1,2-trichloroethane would be 94,000 metric tons (210 million pounds) and 110,000 metric tons (230 million pounds),

respectively assuming a 100% yield. 1,1,2-Trichloroethane is produced by Dow Chemical U.S.A. (Freeport, TX) and PPG Industries, Inc. (Lake Charles, LA) (1, 2). 1,1,2-Trichloroethane is produced primarily as a coproduct of various chlorination processes, such as the production of 1,2-dichloroethane and the chlorination of ethane or 1,1-dichloroethane to produce 1,1,1-trichloroethane (3). 1,1,2-Trichloroethane is also produced when coproduct sources are inadequate or for balancing feedstocks (3). The liquid-phase chlorination of 1,2-dichloroethane is an often used route for producing 1,1,2-trichloroethane (3). 1,1,2-Trichloroethane was found in 9 of 22 commercial batches of technical grade 1,1,1-trichloroethane supplied by eight different European manufacturers and dealers (5). The concentration in these samples ranged from 300 to 3,015 ppm and the detection limit was 0.05 ppm.

[(1) USITC; Synthetic Organic Chemicals. United States Production and Sales, 1991. USITC Publication 2607. pp. 15-33 (1993) (2) SRI International; 1993 Directory of Chemical Producers, United States of America. p. 1006 (1993) (3) Dreher E-L; Ullmann's Encyclopedia of Industrial Chemistry, 5th ed. A6: 275-277, 294-297 (1986) (4) Reed DJ; Kirk-Othmer Encyclopedia of Chemical Technology, 4th ed. 5: 1017-1028 (1993) (5) Henschler D et al; Int Arch Occup Environ Health 47: 263-8 (1980)]

Use: 1,1,2-Trichloroethane is only important as a feedstock intermediate in the production of vinylidene chloride and to some extent in the synthesis of tetrachloroethanes (1, 2). It is also used where its high solvency for chlorinated rubbers and other substances is needed and as a solvent for pharmaceuticals and electronic components (2). However, 1,1,2-trichloroethane's relatively high toxicity does not permit its general use as a solvent (1).

[(1) Dreher E-L; Ullmann's Encyclopedia of Industrial Chemistry, 5th ed. A6: 275-277 (1986) (2) Snedecor G; Kirk-Othmer Encyclopedia of Chemical Technology, 4th ed. 6: 22-24 (1993)]

Occupational Exposure: NIOSH (NOES Survey 1981-83) has statistically estimated that 1,036 workers are potentially exposed to 1,1,2-trichloroethane in the United States (1). The 1974 NIOSH National Occupational Hazard Survey (NOHS) indicated that workers primarily exposed to 1,1,2-trichloroethane were connected with blast furnaces and steel mills, telephone communications, and engineering and scientific instrument manufacture (2). It is not clear if exposure to 1,1,2-trichloroethane in these occupations is from use of the chemical directly or its presence in other products as an impurity. 1,1,2-Trichloroethane was used as an adhesive solvent in a flexible printed circuit factory (no air levels reported) (3) and the garment industry (levels up to 1.0 ppm) (4).

[(1) NIOSH. National Institute for Occupational Safety and Health. National Occupational Exposure Survey (NOES). Computer printout March 29, 1989 (2) IARC. Monographs on the Evaluation of the Carcinogenic Risk of Chemicals to Man. Geneva: World Health Organization, International Agency for Research on Cancer, 1972-present. 20: 536 (1979) (3) Almaguer D, Seligman P; Health Hazard Report No. HETA-84-214-1633, Sheldahl Inc., Northfield MN NIOSH/00179874 (1985) (4) Stayner LT et al; Am J Indust Med 13: 667-81 (1988)]

Consumer Exposure: Information on the use of 1,1,2-trichloroethane in consumer products was not available. In one toxicological case study, the patient was reportedly exposed to 1,1,2-trichloroethane in a waterproofing aerosol (2). Since 1,1,2-trichloroethane may be an impurity in

1,1,1-trichloroethane which is used as a solvent in a wide variety of consumer products (1), consumers may be exposed to 1,1,2-trichloroethane in these products.

[(1) Sack TM et al; Atmos Environ 26A: 1063-1070 (1992) (2) Woo OF et al; J Tox-Clin Toxicol 20: 333-341 (1983)]

Environmental Release and General Population Exposure: According to the 1991 Toxics Release Inventory (TRI), 527,766 pounds of 1,1,2-trichloroethane were released to the environment, of which 99.7% was released into the atmosphere (2). A correlation of data from the EPA Air Toxics Emission Inventory with industrial source categories (SIC codes), shows that emissions of 1,1,2-trichloroethane are associated with plastic materials and resins, industrial organic chemicals, petroleum refining, gaskets-packing and sealing devices, plating and polishing, residential lighting fixtures, radio and TV communication equipment, electronic components, motor vehicle parts and accessories, engineering and scientific instruments, and photographic equipment and supplies (5). It is estimated that emissions from hazardous waste incinerators are 0.11% of 1,1,2-trichloroethane TRI emissions (25). 1,1,2-Trichloroethane has been detected in landfill gas from four municipal landfills with mean concentrations of 0.6 to 8.7 mg/m³ (24).

In a comprehensive survey of wastewater from 4,000 industrial and publicly owned treatment works (POTWs) sponsored by the Effluent Guidelines Division of the EPA, 1,1,2-trichloroethane was identified in discharges of the following industrial category (positive occurrences; median concentration in ppb): timber products (1; 18.46), organics and plastics (1; 7.12), inorganic chemicals (2; 4.00), plastics and synthetics (2; 3.65), auto and other laundries (1; 108.99), organic chemicals (1; 203.77), mechanical products (4; 45.74), transportation equipment (3; 66.34), synfuels (1; 2.43), and POTWs (4; 1.20) (1). The highest effluent concentration was 249.52 ppb in the mechanical products industry (1). According to the TRI, 1,382 pounds of 1,1,2-trichloroethane were released to water and another 819 pounds were released to POTWs (2). 1,1,2-Trichloroethane was detected in 2.8% of 1345 EPA STORET effluent stations at a median concentration below 2.0 ppb (3). Positive identification was made for 1 of 13 effluent samples collected from a community septic tank serving 97 homes near Tacoma, WA (4).

An evaluated database of U.S. air monitoring data for the years 1970-1987 (886 samples) shows the median 1,1,2-trichloroethane concentration as not detectable and 25% of the samples exceeding 0.026 ppb (8). The median and maximum concentration of 1,1,2-trichloroethane in urban/suburban areas of the U.S. (930 samples) were 0.0091 and 11.0 ppb, respectively (6). 1,1,2-Trichloroethane appears to be of anthropogenic origin since it was not detected in rural and remote areas (2 samples), while in source-dominated areas of the U.S. (91 samples), the median, 75th percentile, and maximum concentration were 0.092, 0.210, and 2.3 ppb, respectively (6). In one urban area, Lake Charles, LA, the median concentration was 4.8 ppb (6). The geometric mean concentration of 1,1,2-trichloroethane in three New Jersey Cities, Newark, Elizabeth, and Camden, in 1981/1982 were all 0.01 ppb with 27% of samples positive in the summer and 0.02 to 0.05 ppb with 40% of samples positive in the winter (7). The average 1,1,2-trichloroethane concentration upwind and downwind from a nuclear processing plant in Colorado was 0.007 and 0.011 ppb, respectively (9).

In EPA's Groundwater Supply Survey, none of the 945 finished water supplies that use groundwater sources contained 1,1,2-trichloroethane at a quantification limit of 0.5 ppb (11). 1,1,2-Trichloroethane has been detected in drinking water from samples of U.S. cities (12, 13, 14) with 0.1-8.5 ppb being measured in the finished water from one supply (13). In New York State surveys, wells contained a maximum 1,1,2-trichloroethane concentration of 20 (15) and 13 ppb (23). In a study of thirty Canadian water treatment facilities, 2 were positive for 1,1,2-trichloroethane (7 ppb maximum) in the August/September sampling, but none were positive in the November/December sampling (16).

1,1,2-Trichloroethane was detected in 2 of 13 groundwater samples from Minnesota at levels of 7.7 and 31 ppb (17). In both cases, the contamination was associated with leaching from waste sites. In a groundwater survey in New Jersey, 1,1,2-trichloroethane was found in 72 of 1069 samples with a maximum level of 31.1 ppb (18, 19). Some of the most polluted samples were from urban land use areas.

1,1,2-Trichloroethane was detected in 2% of 1047 EPA STORET water stations (3). In representative New Jersey surface waters, 8.8% of the 603 samples contained 1,1,2-trichloroethane with a maximum level of 18.7 ppb (18). Three of 7 samples from two tributaries of Ohio River contained 1,1,2-trichloroethane with a maximum of 0.6 ppb (21). However, only 4% of the samples from the Ohio River mainstream were positive and 1,1,2-trichloroethane was not found in 88 additional stations. 1,1,2-Trichloroethane has been qualitatively detected in the sediment/soil/water matrix of the Love Canal waste site near Niagara, NY (22).

1,1,2-Trichloroethane was not detected in any of the 46 composite human adipose samples analyzed as part of EPA's National Human Adipose Tissue Survey (NHATS) for fiscal year 1982 (20). Five of 49 breath samples from nine New Jersey subjects in EPA's Total Exposure Assessment Methodology (TEAM) pilot study contained trace to $5.13 \mu\text{g}/\text{m}^3$ of 1,1,2-trichloroethane, with a median of $0.2 \mu\text{g}/\text{m}^3$ (10). All but 10 of the personal air samples from these subjects were below the detection limit, 7 contained trace levels and the others ranged from 0.14 to $34.70 \mu\text{g}/\text{m}^3$ (10).

[(1) Shackelford WM et al; *Analyt Chim Acta* 146: 15-27 (supplemental data) (1983) (2) U.S. EPA; Toxics Release Inventory (1992) (3) Staples CA et al; *Environ Toxicol Chem* 4: 131-42 (1985) (4) DeWalle TB et al; Determination of toxic chemicals in effluent from household septic tanks EPA-600/S2-85-050 (1985) (5) Pacific Environmental Services; Toxic air pollutant/ source crosswalk - A screening tool for locating possible sources emitting toxic air pollutants. EPA-450/4-87-023a (1987) (6) Brodzinsky R, Singh HB; Volatile organic chemicals in the atmosphere: an assessment of available data. SRI International Contract 68-02-3452 Menlo Park, CA: Atmos Sci Ctr 198 p. (1982) (7) Harkov R et al; Volatile organic compounds at urban sites in New Jersey. pp. 69-88 In: Toxic Air Pollution. Chelsea, MI: Lewis Publ Inc (1987) (8) Shah JJ, Heyerdahl; National ambient volatile organic compounds (VOCs) database update. EPA/600/3-88-010(a). Research Triangle Park, NC: EPA p. 49 (1988) (9) Sturges WT, Taylor BE; *Environ Technol* 11: 1063-70 (1990) (10) Wallace LA et al; *Environ Res* 35: 293-319 (1984) (11) Westrick JJ et al; *J Amer Water Works Assoc* 76: 52-9 (1984) (12) IARC; Some halogenated hydrocarbons 20: 533-43 (1979) (13) U.S. EPA; Ambient Water Quality Criteria for Chlorinated Ethanes. EPA-440/5-80-029 p. C-7 (1980) (14) Keith LH et al; Identification and analyses of organic pollutants in water. Ann Arbor, MI: Ann Arbor Press p. 329-73 (1976) (15) Burmaster DE; *Environ* 24: 6-13, 33-6 (1982) (16) Otson R et al; *J Assoc Off Anal Chem* 65: 1370-4 (1982) (17) Sabel GV, Clark TP; *Waste Manage Res* 2: 119-30 (1984) (18) Page GW; *Environ Sci Technol* 15: 1475-81 (1981) (19) Greenberg M et al; *Environ Sci Technol* 16: 14-9 (1982) (20) Stanley JS; Broad scan analysis of the FY82 national human adipose tissue survey specimens.

Volume I - Exec Sum. EPA-560/5-86-035 p. 5 (1986) (21) Ohio River Valley Water Sanit Comm; Assessment of water quality conditions. Ohio River Mainstream 1978-9 Cincinnati, OH (1980) (22) Hauser TR, Bromberg SM; Environ Monit Assess 2: 249-72 (1982) (23) Zaki MH; Northeast Environ Sci 5: 15-22 (1986) (24) Assmuth T, Kalevi K; Chemosphere 24: 1207-1216 (1992) (25) Dempsey CR; J Air Waste Manage Assoc 43: 1374-9 (1993)]

Environmental Transport and Persistence:

Bioaccumulation: The log BCF of 1,1,2-trichloroethane in fish was reported to be <1 (1). Therefore, 1,1,2-trichloroethane would not be expected to bioconcentrate in fish.

[(1) Kawasaki M; Ecotoxicol Environ Safety 4: 444-54 (1980)]

Volatilization/ Adsorption: According to a simple fugacity model, 1,1,2-trichloroethane will distribute almost entirely to air (97.9%); 2.1% will be distribute to water and 0.01% to soil (3). Using the Henry's Law constant, the volatilization half-life for 1,1,2-trichloroethane from a model river 1 m deep with a current of 1 m/s and a wind of 3 m/s is estimated to be 4.6 hours (1). Similarly, the volatilization half-life for a model lake 1 m deep with a 0.05 m/s current and 0.5 m/s wind is 4.9 days. Experimental soil adsorption coefficients, K_{oc} , for 1,1,2-trichloroethane ranged from 83 to 111 in a silty clay soil and 174 to 209 in a sandy loam soil (5). 1,1,2-Trichloroethane moved readily through a column of sandy soil having a retardation factor (velocity of water through the soil divided by the velocity of pollutant) of <1.5 and a K_{oc} of about 70 (6). A K_{oc} of 68 is predicted on the basis of molecular structure (4). The K_{oc} values suggest that 1,1,2-trichloroethane is moderately to highly mobile in soil (2).

[(1) Lyman WJ et al; Handbook of Chemical Property Estimation Methods New York, NY: McGraw-Hill p. 4-9 to 4-10, 15-1 to 15-32 (1982) (2) Swann RL et al; Res Rev 85: 17-28 (1983) (3) U.S. EPA; PCGEMS (Graphical Exposure Modeling System), PCENPART (Environmental Partitioning Model) (4) Meylan WM et al; Environ Sci Technol 26: 1560-7 (1992) (5) Gan DR, Dupont RR; Haz Waste Haz Mat 6: 363-83 (1989) (6) Wilson JT et al; J Environ Qual 10: 501-6 (1981)]

Persistence: 1,1,2-Trichloroethane reacts with photochemically-produced hydroxyl radicals in the atmosphere with a rate constant of $3.24 \times 10^{-13} \text{ cm}^3/\text{molecule-s}$ (1). Assuming a hydroxyl radical concentration of $5 \times 10^5 \text{ radicals/cm}^3$, the half-life of 1,1,2-trichloroethane in the atmosphere will be 32 days. Its disappearance is much faster under simulated smog conditions, the half-life being 16 hours (10). The neutral and basic aqueous hydrolysis rate constants for 1,1,2-trichloroethane at 25 °C have been experimentally determined to be $5.19 \times 10^{-11} \text{ min}^{-1}$ and 0.0942 L/mole-min, respectively, which correspond to half-lives of 139.2 years at pH 7 and 1.39 years at pH 9 (5). 1,1,2-Trichloroethane appears to be resistant to biodegradation under aerobic conditions. It showed no biodegradation in both a 24-day modified shake flask test and a river die-away test (2). Similar results were obtained in another screening biodegradability test (4). When a solution containing 1,1,2-trichloroethane was applied to a column filled with sandy soil, no loss could be attributed to biodegradation (3). No removal as a result of biodegradation was found during wastewater treatment (11). 1,1,2-Trichloroethane has

been shown to undergo biotransformation under methanogenic conditions when it was incubated in the presence of air and methane in a sandy soil (7). Biotransformation of 1,1,2-trichloroethane to vinyl chloride has been observed in screening studies under anaerobic conditions (8). After one week of incubation with 10 ppm of 1,1,2-trichloroethane in an anaerobic digester designed to simulate conditions in a landfill, 0.44 ppm of vinyl chloride was formed, the highest level of any of the chlorinated ethanes and ethenes investigated. Biodegradation of 1,1,2-trichloroethane in groundwater or subsurface regions may occur, but appears to be very slow. No 1,1,2-trichloroethane degradation occurred in soil samples from a 1.2, 3.0, or 5.0 m depth at the margin of a floodplain over a 16 week incubation period (9). The depth to the water table was 3.6 m. The estimated half-life of 1,1,2-trichloroethane in anaerobic groundwater is estimated to be 335 days (6).

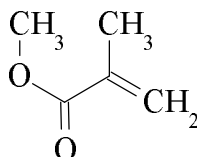
[(1) Atkinson R; J Phys Chem Ref Data. Monograph 1 (1989) (2) Mudder TI, Musterman JL; Amer Chem Soc Div Environ Chem Presentation Kansas City, MO September 1982 p. 52-3 (1982) (3) Wilson JT et al; J Environ Qual 10: 501-6 (1981) (4) Kawasaki M; Ecotoxicol Environ Safety 4: 444-54 (1980) (5) Jeffers PM et al; Environ Sci Technol 23: 965-9 (1989) (6) VanBeelen P; Stygologia 5: 199-212 (1990) (7) Henson JM et al; J Indust Microb 4: 29-35 (1989) (8) Hallen RT et al; ACS Div Environ Chem 192nd National Meeting 26: 344-6 (1986) (9) Wilson JT et al; Ground Water 21: 134-42 (1983) (10) Dilling WL et al; Environ Sci Technol 10: 351-6 (1976) (11) Bhattacharya SK et al; Removal and fate of RCRA and CERCLA toxic organic pollutants in wastewater treatment. EPA-600/2-89-026. Cincinnati, OH: U.S. EPA, Risk Reduction Engineering Lab. (1990)]

METHYL METHACRYLATE

SUBSTANCE IDENTIFICATION

Synonyms: Methyl 2-methyl-2-propenoate; MME; acrylic acid, 2-methyl-, methyl ester;
2-methyl-2-propenoic acid, methyl ester

Structure:



CAS Registry Number: 80-62-6

Molecular Formula: C₅H₈O₂

CHEMICAL AND PHYSICAL PROPERTIES

Boiling Point: 100-101 °C

Melting Point: -48 °C

Molecular Weight: 100.13

Dissociation Constants: Not applicable

Log Octanol/Water Partition Coefficient: 1.38 (1)

Water Solubility: 15,600 mg/L @ 20 °C (2)

Vapor Pressure: 38.4 mm Hg @ 25 °C (3)

Henry's Law Constant: 3.24 x 10⁻⁴ atm-m³/mole (calculated from vapor pressure and water solubility)

Lower Explosive Limit: 2.1% @ 20 °C (4)

[(1) Hansch C, Leo AJ; Medchem Project Issue No 26 Claremont, CA: Pomona College (1985) (2) Riddick JA et al; Organic Solvents 4th ed; New York, NY: Wiley (1986) (3) Daubert TE, Danner RP; Data Compilation Tables of Properties of Pure Compounds American Institute of Chemical Engineering (1985) (4) ACGIH; Documentation of TLVs 5th Edition, p. 406 (1986)]

EXPOSURE PROFILE

Production: There were 1,200 million pounds of methyl methacrylate produced in 1990 of which 135 million pounds were exported (1). Methyl methacrylate is produced by Rohm and Haas (Deer Park, TX), DuPont (Memphis, TN), and Cyro Industries (Fortier, LA) (1).

[(1) Chemical Marketing Reporter; Chemical Profile: Methyl methacrylate. January 14, 1991]

Use: Methyl methacrylate is an acrylic resin monomer (2). It is used for cast and extruded sheet (24%), molded powders and resins (21%), surface coatings (18%), impact modifiers (10%), emulsion polymers (8%), mineral-based sheet (3%), higher methacrylates (2%), and polyester modifiers (1%). Miscellaneous uses, including synthetic fiber modification, consume 2% of production and exports amount to 11% of production (1).

[(1) Chemical Marketing Reporter; Chemical Profile: Methyl methacrylate. January 14, 1991 (2) Hawley CG; The Condensed Chemical Dictionary 10th ed New York, NY: Van Nostrand Reinhold Co (1981)]

Occupational Exposure: NIOSH (NOES Survey 1981-83) has statistically estimated that 120,778 workers are exposed to methyl methacrylate in the United States (5).

In five polymethylmethacrylate sheet manufacturing plants, 8-hour time weighted average (TWA) exposure levels were 4-88 ppm (1). In a polystyrene production plant, TWA breathing zone concentrations and workplace area concentrations were 66 and 169 ppb, respectively, with maximum concentration levels of 378 and 3,300 ppb, respectively (2).

Methyl methacrylate may occur at concentrations below the hygienic threshold limit in dental work rooms and in operating rooms during total hip replacement surgery (3, 4). Dental technicians working with acrylics had methyl methacrylate in their urine (6). In a Russian study, the methyl methacrylate concentration above surfaces freshly painted with commercial acrylic latexes was 1,075 ppb (1).

[(1) IARC; Some Monomers, Plastics and Synthetic Elastomers, and Acrolein; 19: 187-211 (1979) (2) Samimi B, Falbo L; Amer Indust Hyg Assoc J 43: 858-62 (1982) (3) Vedel P et al; Ugeokr Laeg 143: 2734-5 (1981) (4) Brune D, Beltesbrenke H; Scan J Dent Res 89: 113-6 (1981) (5) NIOSH. National Institute for Occupational Safety and Health. National Occupational Exposure Survey (NOES). Computer printout March 29, 1989 (6) Rajaniemi R et al; Brit J Indust Med 46: 356-357 (1989)]

Consumer Exposure: Methyl methacrylate is commonly used in acrylic bone cements and dental devices. Residual methyl methacrylate monomer has been detected in commercial polystyrene copolymer plastics at 36 ppm (1). Residual methyl methacrylate in 5 commercial acrylic bone cements has been reported to have migrated into prepared tissue medium and concentrations as high as 0.7-5.1 weight % were detected in fatty components of bone marrow (1).

[(1) IARC; Some Monomers, Plastics and Synthetic Elastomers, and Acrolein; 19: 187-211 (1979)]

Environmental Release and General Population Exposure: According to the 1991 Toxics Release Inventory (TRI), 2.8 million pounds of methyl methacrylate were released to the environment, of which 90% was released into the atmosphere (1).

It has been demonstrated that methyl methacrylate monomer can migrate from the polymethyl methacrylate into ethanolic solutions at room temperature or into water at elevated temperatures (2). Therefore, there is a potential for methyl methacrylate to migrate into food from polymethylmethacrylate packaging material. Methyl methacrylate has been detected in

commercial deionized charcoal-filtered water (3). It was suggested that the methyl methacrylate may have originated from the plastics used in the preparation or storage of the ion-exchange resin or charcoal (3).

Methyl methacrylate has been detected in Lake Michigan, near Chicago, at 10 ppb (4).

Levels of methyl methacrylate in exhaust stacks from a plant where acrylic resin based paints were dried ranged from 5 to 20 ppm (5). Methyl methacrylate has been detected in combustion products of polymethylmethacrylate (5).

[(1) U.S. EPA; Toxics Release Inventory (1992) (2) Inoue T et al; Bull Nat. Inst Hyg Sci (Tokyo) 144-147 (1981) (3) Dowty BJ et al; Environ Sci Technol 9: 762-5 (1975) (4) Konasewich D et al; Status report on organic and heavy metal contaminants in the lakes Erie, Michigan, Huron, and Superior Basins; Great Lakes Quality Review Board (1978) (5) IARC; Some Monomers, Plastics and Synthetic Elastomers, and Acrolein; 19: 187-211 (1979)]

Environmental Transport and Persistence:

Bioaccumulation: A BCF of 6.6 is estimated for methyl methacrylate from the log K_{ow} (1), indicating a low potential for bioconcentration.

[(1) Lyman WJ et al; Handbook of chemical property estimation methods. Environmental behavior of organic compounds; New York, NY: McGraw-Hill p. 5.5 (Eqn 5-2) (1982)]

Volatilization/ Adsorption: According to a simple fugacity model, methyl methacrylate will distribute entirely to air (1). Using the Henry's Law constant, the volatilization half-life of methyl methacrylate in a model river 1 m deep with a 1 m/s current and a 3 m/s wind speed is estimated to be 5.6 hours (2). Similarly, the volatilization half-life of methyl methacrylate in a model lake 1 m deep with a 0.05 m/s current and 0.5 m/s wind is 4.8 days (2). A K_{oc} of 22 is estimated for methyl methacrylate from its water solubility using a recommended regression equation (2), indicating that little adsorption of methyl methacrylate to soil should occur. In view of its high vapor pressure, high Henry's Law constant, and low adsorptivity to soil, methyl methacrylate would be expected to volatilize rapidly from soil.

[(1) U.S. EPA; PCGEMS (Graphical Exposure Modeling System), PCENPART (Environmental Partitioning Model) (2) Lyman WJ et al; Handbook of chemical property estimation methods. Environmental behavior of organic compounds; New York, NY: McGraw-Hill pp. 4-9 (Eqn 4-5), 15.1 to 15.34 (1982)]

Persistence: Methyl methacrylate is readily polymerized by light and heat (1); therefore, an inhibitor, generally 10-15 ppm of the monomethyl ester of hydroquinone, is added to it (2). Hydrolysis of simple esters is slow (4). The estimated basic hydrolysis rate constant for methyl methacrylate is 3.4×10^{-3} L/mol-sec (5). The hydrolysis half-life at pH 8 would therefore be 6.5 years.

Methyl methacrylate will react with both hydroxyl radicals and ozone in the atmosphere with respective estimated rate constants of $47.1 \times 10^{12} \text{ cm}^3/\text{molecule-s}$ and $1.14 \times 10^{17} \text{ cm}^3/\text{molecule-s}$ (6). Assuming a hydroxyl radical concentration of $5 \times 10^5 \text{ radicals/cm}^3$ and an ozone concentration of $7 \times 10^{11} \text{ molecules/cm}^3$, the half-life of methyl methacrylate in the atmosphere with respect to hydroxyl radical and ozone attack, will be 8.1 hours and 24 hours, respectively. Methyl methacrylate is moderately reactive in a smog chamber (3). With methyl methacrylate and nitrogen oxides concentration ratios typical of urban areas, the photodegradation half-life was 2.7 hours; the half-life exceeded 3 hours when the concentration ratios were typical of rural areas (3).

Methyl methacrylate is readily biodegradable according to laboratory tests using a mixed inoculum of soil, surface water, and sewage and activated sludge and sewage inocula (7-9).

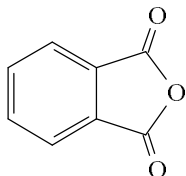
[(1) Hawley; Condensed Chemical Dictionary (1981) (2) Kirk-Othmer Encyclopedia of Chemical Technology; 3rd ed; Wiley; 15: 346-76 (1981) (3) Joshi SB et al; Atmos Environ 16: 1301-10 (1982) (4) Mabey W, Mill T; J Phys Chem Ref Data 7: 383-415 (1978) (5) U.S. EPA; PCGEMS (Graphical Exposure Modeling System), PCHYDRO (6) Meylan WM, Howard PH; Chemosphere 26: 2293-2299 (1993) (7) Sasaki S; pp. 283-98 In: Aquatic pollutants: Transformation and biological effects. Hutzinger O et al. eds; Pergamon Press (1978) (8) Slave T et al; Rev Chim 25: 666-70 (1974) (9) Pahren HR, Bloodgood DE; Water Pollut Control Fed J 33: 233-8 (1961)]

PHTHALIC ANHYDRIDE

SUBSTANCE IDENTIFICATION

Synonyms: 1,2-Benzenedicarboxylic acid anhydride; PA

Structure:



CAS Registry Number: 85-44-9

Molecular Formula: C₈H₄O₃

CHEMICAL AND PHYSICAL PROPERTIES

Boiling Point: 295 °C, sublimes

Melting Point: 130.8 °C

Molecular Weight: 148.11

Dissociation Constants: Not applicable

Log Octanol/Water Partition Coefficient (log K_{ow}): (See note below)

Water Solubility: 6200 ppm @ 25 °C (2)

Vapor Pressure: 2 x 10⁻⁴ mm Hg @ 20 °C (1); 6.0 mm Hg @ 132 °C (3)

Henry's Law Constant: 6.2 x 10⁻⁹ atm-m³/mole (calculated from vapor pressure and water solubility)

Lower Explosive Limit: Not available

Note: Data in the literature concerning the physical/chemical properties of phthalic anhydride are inconsistent. Phthalic anhydride reportedly hydrolyzes in water with a half-life of <30 minutes (references 2, 5, and 7 from persistence), but has a measured water solubility of 6200 ppm (2) and a measured bioconcentration factor (reference 1 from bioaccumulation). The aqueous hydrolysis of phthalic anhydride is a reversible process (2), but no detailed description of this equilibrium was found in the literature. Because of this and the reported rapid hydrolysis, the water solubility and bioconcentration factors may be suspect.

[(1) Verscheuren K; Handbook of Environ Data on Organic Chemicals, 2nd ed. p. 1002 Van Nostrand Reinhold (1983) (2) Towle PH et al; Kirk-Othmer Encyclopedia of Chemical Technology 2nd ed. 15: 444 (1968) (3) Bemis AG et al; Kirk-Othmer Encyclopedia of Chemical Technology, 3rd ed. 17: 732-777 (1982)]

EXPOSURE PROFILE

Production: There were 874 million pounds of phthalic anhydride produced in 1991 of which 77.7 million pounds were exported; an additional 27.9 million pounds were imported (1). Phthalic anhydride is produced by Exxon (Baton Rouge, LA), Aristech (Pasadena, TX), Koppers (Cicero, IL), Stepan (Millsdale, IL), and Sterling (Texas City, TX) (1).

[(1) Chemical Marketing Reporter; Chemical Profile: Phthalic Anhydride. August 10, 1992]

Use: Phthalic anhydride is primarily used in the production of plasticizers (54%) (1). It is also used in the production of unsaturated polyester resins (21%), and alkyd resins (17%) (1). Miscellaneous uses, including dyes, pigments, and polyester polyols, consume 8% of production (1). The overwhelming majority of alkyd resins are based on phthalic anhydride; they are composed of <20% to >35% phthalic anhydride (2). Phthalic anhydride is used as a curing agent for epoxy resins that have important coating and structural applications (3).

[(1) Chemical Marketing Reporter; Chemical Profile: Phthalic Anhydride. August 10, 1992 (2) Lin KF; Kirk-Othmer Encyclopedia of Chemical Technology, 4th ed. 2: 54-55 (1992) (3) Muskopf JW, McCollister SB; Ullmann's Encyclopedia of Industrial Chemistry A9: 555-557 (1987)]

Occupational Exposure: NIOSH (NOES Survey 1981-83) has statistically estimated that 62,644 workers are exposed to phthalic anhydride in the United States (1). Time-weighted average (TWA) concentrations of phthalic anhydride ranging from 4 to 203 $\mu\text{g}/\text{m}^3$ were found in a facility that manufactured phthalic anhydride, produced diethyl-hexyl phthalate (DEHP), and pumped phthalic anhydride into tankcars and trucks for shipment (7). Workers in another plant that manufactured phthalic anhydride and used phthalic anhydride to produce unsaturated polyester resins were exposed to phthalic anhydride TWA levels of 0.03 to 10.5 mg/m^3 . Urine levels of phthalic anhydride correlated with exposure and ranged from 0.3 to 14.0 $\mu\text{mol}/\text{mmol}$ creatine (11). In facilities that use phthalic anhydride, such as one alkyd and unsaturated polyester resin production plant, workers are sometimes required to cut open and manually empty bags of flaked phthalic anhydride into a chemical reactor (9, 14). In such situations, there is a high probability of exposure to phthalic anhydride dust. When used as curing agent for epoxy resins, most anhydrides require elevated temperatures (2). With DGEBA (diglycidyl ether of bisphenol A), it is recommended to heat the resin to 120 °C to 140 °C, followed by the addition of phthalic anhydride, and then let the mixture cool to 60 °C (2). During this process, some of the phthalic anhydride sublimes. There would be a potential for occupational exposure during this procedure.

Phthalic anhydride is a thermal decomposition product of PVC soft wrap and price label adhesive (3, 10). On heating, phthalic anhydride was emitted as vapor, fume, and dust from diethylhexyl phthalate (DEHP) and three polyvinyl plastics containing phthalates (12). Phthalic anhydride emissions increased with increasing temperature. Phthalic anhydride vapors emitted during heat sealing plastic films on meat are believed to be responsible for meatwrapper's asthma (3, 10). The air level of phthalic anhydride in a meat department of a supermarket was 18.4 ppm (4). Phthalic anhydride is the main thermal degradation product of alkyd paints (5, 6) and therefore, it may be emitted during welding or flame cutting painted steel and other metals. Phthalic anhydride in the bulk residue of the compressed air system of a factory investigated for health complaints was a

possible thermal decomposition product of the synthetic compressor oil (8). Area samples collected in nine Finnish PVC plastics processing plant during extrusion, calendaring, hot embossing, welding, injection molding, compounding, thermoforming, high frequency welding, spread coating, blow molding, and compression molding contained between 0.02 and 5.0 µg/m³ of phthalic anhydride (13).

[(1) NIOSH. National Institute for Occupational Safety and Health. National Occupational Exposure Survey (NOES). Computer printout March 29, 1989 (2) Lee H, Neville K; Handbook of Epoxy Resins pp. 12-2 and 12-16 New York, NY: McGraw Hill Book Company (1982) (3) Bardana EJ Jr; Meatwrapper's asthma: Clinical and pathological observations. pp. 14-32 In: Occupational Asthma, CA Frazier ed, New York, NY: Van Nostrand Reinhold (1980) (4) Daniels WJ et al; Health Hazard Evaluation Report No. HETA-84-2399-1586, Ashland Super Valu, Ashland, Wisconsin. NIOSH, Cincinnati, OH (1985) (5) Henriks-Ekerman ML et al; Am Indust Hyg Assoc J; 51: 241-244 (1991) (6) Leleu J; Cashiers de Notes Documentaires 100: 383-388 (1980) (7) Liss GM et al; Scand J Work Environ Health 11: 381-387 (1985) (8) McQuilkin SD, Shea L; Health Hazard Evaluation Report No. HETA-79-49-631, Dana Corporation, Spicer Universal Joint Division, Marion, Indiana. NIOSH, Cincinnati, OH (1979) (9) Nielsen J et al; J Allergy Clin Immunol 82: 126-132 (1988) (10) Pauli G et al; Clin Allergy 10: 263-269 (1980) (11) Pfaffli P; Int Arch Occup Environ Health 58: 209-216 (1986) (12) Pfaffli P; Analyst 111: 813-817 (1986) (13) Vainiotalo S, Pfaffli P; Ann Occup Hyg 34: 585-590 (1990) (14) Weernfors M et al; Int Arch Allergy Appl Immunol 79: 77-82 (1986)]

Consumer Exposure: No information was found which would indicate that phthalic anhydride is used in consumer products. One use that would appear to have a potential for consumer exposure is as a curing agent for epoxy resins. However, most anhydride curing agents require elevated temperatures. Therefore, phthalic anhydride is not likely to be used in consumer epoxy resins that cure at room temperature (1). Phthalic anhydride may be emitted from PVC plastics on heating (see Occupational Exposure). Consumers of PVC film who use heat sealers may therefore be exposed to phthalic anhydride.

[(1) Lee H, Neville K; Handbook of Epoxy Resins pp. 12-2, 12-16 New York, NY: McGraw Hill Book Company (1982)]

Environmental Release and General Population Exposure: According to the 1991 Toxics Release Inventory (TRI), 645,932 pounds of phthalic anhydride were released to the environment, of which 98% was released into the atmosphere (1). Since phthalic anhydride may be formed when phthalate-containing material, such as PVC plastics, are heated (see Occupational Exposure), incineration of industrial and municipal refuse and sludges may produce phthalic anhydride emissions. Phthalic anhydride was identified, but not quantified, in urban air particles collected in St. Louis, MO over an 18 month period (2).

[(1) U.S. EPA; Toxics Release Inventory (1992) (2) Ramdahl T et al; Environ Sci Technol 16: 861-5 (1982)]

Environmental Transport and Persistence:

Bioaccumulation: Phthalic anhydride did not bioconcentrate in *Daphnia magna*, *Physa* (snail), or *Gambusia* (fish), but had a reported bioconcentration factor of 200 in *Oedogonium* (alga) (1). Analysis was made by thin layer chromatography. It is possible that a co-eluting degradation product could have been confused for phthalic anhydride.

[(1) Lu PY, Metcalf RL; Environ Health Perspect 10: 269-84 (1975)]

Volatilization/ Adsorption: According to a simple fugacity model, the mass distribution of phthalic anhydride among the environmental compartments at equilibrium (ignoring hydrolysis) is 0.9850 to water, 0.0146 to air, and 0.0004 to soil (3). Phthalic anhydride's very low Henry's Law constant indicates that it would not volatilize from surface waters before it hydrolyzes (2). Phthalic anhydride is estimated to have low adsorptivity to soil. The K_{oc} for phthalic anhydride estimated from its water solubility and assuming no hydrolysis, using a recommended regression equation, is 36 (2). The K_{oc} estimated from molecular structure is 11 (1). Due to its low vapor pressure and low Henry's law constant and apparent ready hydrolysis, volatilization from dry and moist soil should be minimal.

[(1) Meylan WM et al; Environ Sci Technol 26: 1560-1567 (1992) (2) Lyman WJ et al; Handbook of Chemical Property Estimation Methods. Environmental Behavior of Organic Compounds. New York, NY: McGraw Hill pp. 4.9 (Eqn 4-5), 15.1-15.34 (1982) (3) U.S. EPA; PCGEMS (Graphical Exposure Modeling System), PCENPART (Environmental Partitioning Model)]

Persistence: Phthalic anhydride hydrolyzes in water. The hydrolysis rate is $7.9 \times 10^{-3} \text{ s}^{-1}$ at 25 °C (2), indicating a half-life of phthalic anhydride in water of 1.5 minutes. In dioxan-water 60:40 (v/v), the hydrolysis rate is $42.9 \times 10^{-5} \text{ s}^{-1}$ (7). In the course of solubilizing and hydrolyzing, half of the phthalic anhydride added to water is converted to phthalic acid in approximately 30 minutes (5). Therefore, in laboratory or industrial situations in which phthalic anhydride is added to water, it may be present for much longer than the hydrolytic half-life in water suggests. Phthalic anhydride absorbs light $>290 \text{ nm}$ (3) and may therefore undergo direct photolysis. When these photolytic reactions were studied in distilled water, river water, and seawater, the phthalic anhydride, which hydrolyzes to phthalic acid, polymerized to polyphenyl with molecular weights ranging from 2,800 to 3,600 (6).

The gas/particle partitioning of semivolatile organic compounds in the atmosphere depends on the vapor pressure of the organic compound and the concentration of total suspended particulate matter (1). According to this theory, atmospheric phthalic anhydride will primarily be found in the vapor phase. As the vapor, it will react with photochemically-produced hydroxyl radicals with an estimated rate constant of $5.04 \times 10^{13} \text{ cm}^3/\text{molecule-s}$ (4). Assuming a hydroxyl radical concentration of $5 \times 10^5 \text{ radicals/cm}^3$, the half-life of phthalic anhydride will be 32 days.

Phthalic anhydride is reported to biodegrade in laboratory tests using sewage and activated sludge inocula (8-11). Results include 33% mineralization in 24 hours (10) and 5-day BOD values of 22-78 (8, 9). The initial step in the biodegradation studies would be the chemical hydrolysis of phthalic anhydride to phthalic acid.

(1) Bidleman T; Environ Sci Technol 22 361-367 (1988) (2) Hawkins MD; J Chem Soc Perkin Trans 2 75: 282-4 (1975) (3) Sadtler UV No. 18 (1966) (4) Atkinson R; J Inter Chem Kinet 19: 799-828 (1987) (5) Setinek K et al; Collection Czech Chem Commun 27: 2694-2699 (1962) (6) Bajt O et al; Chemosphere 24: 673-679 (1992) (7)

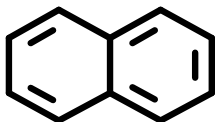
Bunton CA et al; J Chem Soc 1963: 2918-2926 (1963) (8) Heukelekian H, Rand MC; J Water Pollut Contr Assoc 29: 1040-53 (1955) (9) Takemoto S et al; Suishitsu Odaku Kenkyu 4: 80-90 (1981) (10) Matsui S et al; Prog Water Technol 7: 645-59 (1975) (11) Sasaki S; pp. 283-98 In: Aquatic Pollutants: Transformation and Biological Effects Hutzinger O et al. ed. Oxford: Pergamon Press (1978)]

NAPHTHALENE

SUBSTANCE IDENTIFICATION

Synonyms: There are no commonly used synonyms.

Structure:



CAS Registry Number: 91-20-3

Molecular Formula: C₁₀H₈

CHEMICAL AND PHYSICAL PROPERTIES

Boiling Point: 217.9 °C

Melting Point: 80.2 °C

Molecular Weight: 128.16

Dissociation Constants: Not applicable

Log Octanol/Water Partition Coefficient (log K_{ow}): 3.30 (1)

Water Solubility: 31.7 mg/L @ 25 °C (2)

Vapor Pressure: 0.082 mm Hg @ 25 °C (2)

Henry's Law Constant: 4.83 x 10⁻⁴ atm-m³/mole (3)

Lower Explosive Limit: Not available

[(1) Hansch C, Leo AJ; Medchem Project Issue No 26 Claremont, CA: Pomona College (1985) (2) Riddick JA et al; Organic Solvents 4th ed; New York, NY: Wiley (1986) (3) Mackay D et al; Environ Sci Technol 13: 333-336 (1979)]

EXPOSURE PROFILE

Production: There were 235 million pounds of naphthalene produced in 1989; imports were negligible (1). Naphthalene is produced by Koppers (Follansbee, WV), Allied (Ironton, OH), Texaco (Delaware City, DE), and Advanced Aromatics (Baytown, TX) (1). A more recent compilation of naphthalene producers lists only Allied Signal, Inc. (Follansbee, WV and Ironton, OH) and Advanced Aromatics (Baytown, TX) (2).

[(1) Chemical Marketing Reporter; Chemical Profile: Naphthalene. November 5, 1990 (2) SRI International; 1993 Directory of Chemical Producers, United States of America p. 779 (1993)]

Use: Naphthalene is used primarily as a feedstock in the production of phthalic anhydride (55%) (1). It is also used in the production of carbaryl (1-naphthyl-N-methylcarbamate), an insecticide,

and related products (tetralin and 1-naphthol) (12%), dispersant chemical (including superplasticizers) (12%), moth repellent (7%), synthetic tanning agents (4%), miscellaneous (5%), and exports (5%) (1). Naphthalene is also a component of gasoline (2).

Naphthalene is a raw material that is used to produce a number of commercially important chemicals (3). Phthalic anhydride, an intermediate for PVC plasticizers, resins, and insecticides, is made from naphthalene by catalytic vapor-phase oxidation. Naphthalene is a feedstock for the manufacture of 2-naphthol and naphthalene sulfonic acid, which are used as intermediates in the synthesis of azo dyes. The sulfonates of naphthalene and alkylnaphthalene are used as surfactants. Naphthalene sulfonate-formaldehyde condensates find use as tanning agents and dispersants for concrete. It is hydrogenated to produce the solvents tetralin and decalin.

Diisopropylnaphthalenes are used as solvents for carbonless copy paper. Naphthalene is also used to make chemicals that are used as pesticides, plant growth regulators, polyester/polyamide polymers, lube-oil additives, dispersants, flue gas desulfurization, and wood preservatives. Naphthalene itself is used as a moth repellent (3).

[(1) Chemical Marketing Reporter; Chemical Profile: Naphthalene. November 5, 1990 (2) American Petroleum Institute; Gasoline vapor exposure assessment at service stations. API Publication 4553, pp. 1-21, Table D-1, page 15 of 15, July 1991 (1993) (3) Collin H; Ulmann's Encyclopedia of Industrial Chemistry A17: 1-8 (1991)]

Occupational Exposure: NIOSH (NOES Survey 1981-83) has statistically estimated that 23,092 workers are exposed to naphthalene in the United States (1). Polycyclic aromatic hydrocarbons (PAHs), which may include naphthalene, are emitted into the air by most industrial processes involving incomplete combustion of organic materials. Many PAHs so released may be strongly adsorbed to carbonaceous material (5). It is estimated that workers may be exposed to as much as 220 ppm of naphthalene in the vapor phase and up to $4.4 \mu\text{g}/\text{m}^3$ in particulate matter in industry (8). Naphthalene-exposed workers may include those who make β -naphthol, celluloid, dye chemicals, fungicides, hydronaphthalene, lampblack, phthalic anhydride, or smokeless powder, as well as those who work with coal tar, textile chemicals, or moth repellents or those who work in tanneries or aluminum reduction plants (8). Air levels of naphthalene in factories include: an aluminum reduction plant - 0.72 to $311.3 \mu\text{g}/\text{m}^3$ (0.1 to 59.5 ppb) in the vapor phase and 0.090 to $4.00 \mu\text{g}/\text{m}^3$ in particulates (8); coke oven - 11.35 to $1,120 \mu\text{g}/\text{m}^3$ (2 to 214 ppb) in the vapor phase and ND to $4.40 \mu\text{g}/\text{m}^3$ in particulates (8); and silicon carbide plant - 1.3 to $58 \mu\text{g}/\text{m}^3$ (5). The average exposure to naphthalene in particulates and in the vapor phase, respectively, in specified operation in certain industries as determined from field studies are: paving/roofing/steel/silicon carbide - 11.43 and $0.08 \mu\text{g}/\text{m}^3$; refractory brick - 16.30 and ND $\mu\text{g}/\text{m}^3$; silicon carbide - 75.40 and $0.01 \mu\text{g}/\text{m}^3$; and aluminum refinery - $1,111.4$ and $0.52 \mu\text{g}/\text{m}^3$ (3).

Naphthalene was found to be the predominant PAH detected among coke oven workers in a Swedish steel mill, accounting for 60 to 95% of PAH exposures, which ranged from 6 to $570 \mu\text{g}/\text{m}^3$ (7). Heavy soot that may contain naphthalene is produced during the casting process. Naphthalene emissions released at a pilot-scale foundry during aluminum and grey iron casting by the conventional green sand and the new EPC process, which uses low density polystyrene foam

facsimiles of the part to be cast, ranged up to 9,800 µg/kg of metal (4). Naphthalene was detected in a Danish smokehouse where fish was cured over smoldering alder chips at 2,918 µg/m³ (3). Naphthalene was the main organic component in vapors in creosote impregnation plants (6). The mean concentrations of naphthalene in the breathing zone of workers in various job categories in two creosote impregnation plants in Finland ranged from 0.2 to 41 mg/m³ (6). Job categories having the highest levels of exposure were those that cleaned or opened the impregnation chamber. Other exposed workers are those involved in processing, transporting, and installing treated wood products such as railroad ties and telephone poles.

The naphthalene content of ash from municipal refuse incinerators ranged from 1,300 to 28,000 ppb and therefore, workers at an incinerator or workers who transport or dispose of the ash may be exposed to naphthalene (9). Naphthalene is a component of JP-4 and JP-8 jet fuel and workers handling these fuels may be exposed to naphthalene by inhalation or dermal contact (2).

[(1) NIOSH. National Institute for Occupational Safety and Health. National Occupational Exposure Survey (NOES). Computer printout March 29, 1989 (2) Smith JH, Harper JC; 12th Conference on Environmental Toxicology; pp. 336-53 (1982) (3) Nordholm L et al; Scan J Work Environ Health 12: 614-618 (1986) (4) Gressel MG et al; Appl Ind Hyg 3: 11-17 (1988) (5) Dufresne A et al; Am Ind Hyg Assoc J 48: 160-166 (1987) (6) Heikkila PR et al; Scand J Work Environ Health 13: 431-437 (1987) (7) Reuterwall et al; Scand J Work Environ Health 17: 123-132 (1991) (8) U.S. EPA; Ambient Water Quality Criteria: Naphthalene; EPA 440/5-80-059 (1980) (9) Shane BS et al; Arch Environ Contam Toxicol 19: 665-73 (1990) (10) Lesage J et al; Am Ind Hyg Assoc 48: 753-9 (1987)]

Consumer Exposure: Consumers who use naphthalene as a mothproofing agent will be exposed to naphthalene while storing clothing in mothballs or unpacking them. The exposure to naphthalene may be moderately high because clothing would be stored in a confined space and room ventilation may be poor. In a study of customer exposure to gasoline components at 6 service stations in 3 geographical areas, the air concentrations of naphthalene at the stations (12 samples) were all 0.09 ppm, while the naphthalene in samples taken at the perimeter of the stations were all 0.005 ppm (1).

[(1) American Petroleum Institute; Gasoline vapor exposure assessment at service stations. API Publication 4553, pp. 1-21, Table D-1, page 15 of 15, July 1991 (1993)]

Environmental Release and General Population Exposure: According to the 1991 Toxics Release Inventory (TRI), 2.8 million pounds of naphthalene were released to the environment, of which 95.5% was released into the atmosphere, 1.9% to land, and 1.1% to water (1). Worst-case naphthalene emissions from hazardous waste incinerators are estimated to be 2,280 pounds/year (33).

In a comprehensive survey of wastewater from 4,000 industrial and publicly owned treatment works (POTWs) sponsored by the Effluent Guidelines Division of the U.S. EPA, naphthalene was identified in discharges of the following industrial category (positive occurrences; median concentration in ppb): timber products (26; 228.6), leather tanning (1; 27.6), iron and steel mfg (8; 52.4), petroleum refining (14; 312.7), nonferrous metals (6; 25.1), paving and roofing (1; 4.5), paint and ink (26; 174.3), printing and publishing (7; 58.7), ore mining (8; 281.0), coal mining

(23; 50.9), organics and plastics (36; 1574.7), inorganic chemicals (12; 12.1), textile mills (4; 34.4), plastics and synthetics (5; 79.6), pulp and paper (5; 56.9), rubber processing (7; 232.0), auto and other laundries (23; 170.1), pesticides manufacture (6; 487.7), photographic industries (1; 33.4), pharmaceuticals (2; 10.7), explosives (4; 76.9), foundries (24; 13.8), aluminum (7; 44.1), electronics (21; 50.1), oil and gas extraction (18; 69.1), organic chemicals (37; 74.7), mechanical products (25; 439.4), transportation equipment (7; 50.4), amusements and athletic goods (2; 637.2), POTWs (118; 45.5), and rum industry (7; 328.4) (6). Industries that had effluents above 10 ppm (highest effluent concentration in ppm) are: timber products (126.1), organics and plastics (8,837.4), pesticides manufacture (21.4), and mechanical products (46.9) (6). Gaseous effluents from coal-fired power plants under near-ideal conditions contained 0.01 to 1.8 $\mu\text{g}/\text{m}^3$ (24).

Urban air in the U.S. (11 samples) contained a median naphthalene concentration of 180 ppt with a range of 11 to 480 ppt (26). Air in source-dominated areas (95 samples) contained a median naphthalene concentration of 400 ppt with a maximum of 16 ppb (26). Air in Narragansett Bay (coastal), Kingston (urban), and Providence (urban, industrial), RI contained 52.3, 59.0, and 348.7 pg/m^3 of naphthalene, respectively (25). Naphthalene levels in air in residential areas near an aluminum reduction plant ranged from 11.3 to 117 ng/m^3 (23, 30). During air pollution episodes in Torrance and Glendora, CA, the naphthalene levels were 2.9 to 3.3 and 3.1 to 4.3 $\mu\text{g}/\text{m}^3$, respectively (29, 32). Naphthalene levels in air in the Allegheny Mt. Tunnel on the Pennsylvania Turnpike increased with traffic and ranged from 3.5 to 10.1 u/m^3 (27). In homes in the Chicago area, 43% contained detectable concentrations of naphthalene, whereas 21% of outdoor air samples contained naphthalene (28). The average (range) naphthalene levels in twelve Canadian homes and in the ambient air were 13.9 $\mu\text{g}/\text{m}^3$ (1 to 77 $\mu\text{g}/\text{m}^3$) and 2.0 $\mu\text{g}/\text{m}^3$ (ND to 5 $\mu\text{g}/\text{m}^3$), respectively (31).

Naphthalene has been detected in surface water at some sites in Lake Michigan, and the Delaware, Ohio, Charles, and Mississippi Rivers at concentrations up to 34 ppb near industrial sites (7, 8, 9, 10, 11, 12, 13) and 27 ppb 0.67 miles downstream from the site of a tire fire (14). The mean concentration of naphthalene in unpolluted seawater in the Gulf of Mexico was 0.2 ppt (15), while in Vineyard Sound on Cape Cod, MA, the mean was 12 ppt, and the maximum was 35 ppt. The levels displayed a strong seasonal pattern, suggesting input from heating fuels from runoff or the atmosphere (16, 17). Estuarine sites in Texas adjacent to an offshore shallow-water multiwell platform contained 2.1 ppb of naphthalene; 10 m from the platform, the level was 54.7 ppb (18).

Naphthalene in sediment is generally associated with oil spills or industrial effluent. Naphthalene was not detected in sediment in unpolluted areas in the Strait of Juan de Fuca and Northern Puget Sound, WA (22). In Casco Bay, MA, naphthalene was found in 1 of 30 samples tested at 113 ppb (19). Naphthalene levels in sediment (0-6 cm) in Windsor Cove, Buzzards Bay, MA was 9.2 ppm in October 1974 when an oil spill occurred (20). This level decreased to 0.63 ppm in May 1975 and 0.11 ppm in June 1977 (20). Naphthalene levels in sediments (0-5 cm) from sites in Norwegian fjords were: 800 m from a ferro alloy plant - 2,870 ppb; 500 m from an aluminum

plant - 220 ppb; 15 - 20 km from ferro and aluminum plants - 41.5 ppb; 800 m from a petroleum refinery - 70.0 ppb; 500 m and 10 km from a North Sea oil field - 31.6 ppb and 4.32 ppb, respectively; and sites close to Oslo - 45.8 to 53.6 ppb (21). Soil near an aluminum reduction plant contained 48.3 ppm of naphthalene, whereas unpolluted soil contained 46.2 ppb (23).

Naphthalene was not detected in composite samples of fish from Great Lakes harbors and tributary mouths in a 1980-1981 survey (5). In a 1982 survey at Commencement Bay in Puget Sound, WA, the highest concentration of naphthalene in bottom fish was 0.51 ppm (4).

Naphthalene was detected in 6 of 8 samples of mother's milk from four urban areas (2). Naphthalene was detected in 40% of adipose tissue analyzed in the National Human Adipose Tissue Survey (NHATS) by EPA for fiscal year 1982 at levels ranging from <9 ppb to 63 ppb wet weight (3).

[(1) U.S. EPA; Toxics Release Inventory (1992) (2) Pellizzari ED et al; Bull Environ Contam Toxicol 28: 322-8 (1982) (3) Stanley JS; Broad scan analysis of the FY82 national human adipose tissue survey specimens Volume III. Semi-volatile organic compounds EPA-560/5-860-037, Washington, DC pp. 148 (1986) (4) Nicola RM et al; J Environ Health 49: 342-7 (1987) (5) DeVault DS; Arch Environ Contam Toxicol 14: 587-94 (1985) (6) Shackelford WM et al; Analyt Chim Acta 146: 15-27 (supplemental data) (1983) (7) Sheldon LS, Hites RA; Environ Sci Technol 12: 1188-94 (1978) (8) Jungclaus GA et al; Environ Sci Technol 12: 88-96 (1978) (9) Ohio River Valley Water Sanit Comm; Assessment of water quality conditions Ohio River Mainstreams 1978-9 Cincinnati OH (1980) (10) Hites RA, Biemann K; Science 178: 158-60 (1972) (11) Sheldon LS, Hites RA; Environ Sci Technol 13: 574-9 (1979) (12) Konasewich D et al; Status report on organic and heavy metal contaminants in the Lake Erie, Michigan, Huron, and Superior Basins. Great Lakes Quality Board; pp. 273 (1978) (13) DeLeon IR et al; Chemosphere 15: 795-805 (1986) (14) Peterson JC et al; Anal Chem 58: 70A-74A (1986) (15) Sauer TC Jr; Org Geochem 3: 91-101 (1981) (16) Gschwend PM et al; Environ Sci Technol 16: 31-8 (1982) (17) Mantoura RFC et al; Environ Sci Technol 16: 38-45 (1982) (18) Brooks JM et al; Environ Sci Technol 24: 1079-85 (1990) (19) Larsen PF et al; Bull Environ Contam Toxicol 30: 530-5 (1983) (20) Teal JM et al; J Fish Res Board Canada 35: 510-20 (1978) (21) Sporstoe S et al; Environ Sci Technol 17: 282-6 (1983) (22) Brown DW et al; Investigation of petroleum in the marine environs of the Strait of Juan de Fuca and Northern Puget Sound; p. 33 EPA-600/7-79-164 (1979) (23) Vogt NB et al; Environ Sci Technol 21: 35-44 (1987) (24) Junk GA et al; ACS Symp Ser 319 (Fossil Fuels Utilize) pp. 109-23 (1986) (25) Krstulovic AM et al; Am Lab 9: 11-8 (1977) (26) Brodzinsky R, Singh HB; Volatile Organics in the Atmosphere: An Assessment of Available Data p. 198 SRI 68-02-3452 (1982) (27) Hampton CV et al; Environ Sci Technol 17: 699-708 (1983) (28) Jarke FH et al; ASHRAE Trans 87: 153-66 (1981) (29) Arey J et al; Atmos Environ 21: 1437-45 (1987) (30) Thrane KE; Atmos Environ 21: 617-28 (1987) (31) Chan CC et al; J Air Waste Manage Assoc 40: 62-7 (1990) (32) Arey J et al; Environ Sci Technol 23: 321-7 (1989) (33) Demspey CR; Air & Waste 43: 1374-1379 (1993)]

Environmental Transport and Persistence:

Bioaccumulation: Naphthalene bioconcentrates to a moderate extent in fish and aquatic invertebrates (log BCF 1.6-3.0) (1-6). At least for invertebrates, depuration is rapid when the organism is placed in water free of the pollutant (6, 7). Some marine organisms have no detectable aryl hydrocarbons hydroxylase enzyme systems, namely: phytoplankton, certain zooplankton, mussels (*Mytilus edulis*), scallops (*Placopecten sp*), and snails (*Littornia littorea*). Those organisms, which lack a metabolic detoxification enzyme system, would tend to accumulate naphthalene. Naphthalene is readily metabolized in fish (8) which should limit bioaccumulation.

[(1) Roubal WT et al; Arch Environ Contam Toxicol 7: 237-44 (1978) (2) Veith GD et al; J Fish Res Board Canada 36: 1040-8 (1979) (3) Southworth GR et al; Water Res 12: 973-7 (1978) (4) Geyer H et al; Chemosphere 11: 1121-34 (1982) (5) Lee RF; pp. 60-70 In: Fate and Effects of Petroleum Hydrocarbons in Marine Organisms and Ecosystems Volume 6. Wolfe DA ed. (1977) (6) Eastmond DA et al; Arch Environ Contam Toxicol 13: 105-11 (1984) (7) Tarshis IB; Arch Environ Contam Toxicol 10: 79-86 (1981) (8) Callahan MA et al; Water-related environmental fate of 129 priority pollutants; pp. 95-1 to 95-20 EPA-440/4-79-029b (1979) (9) Malins DC; Ann NY Acad Sci 298: 482-496 (1977)]

Volatilization/ Adsorption: According to a simple fugacity model, the mass distribution of naphthalene among the environmental compartments at equilibrium is 0.9987 in air, 0.0012 in water, and 0.0001 in soil (21). The estimated half-life for the volatilization of naphthalene from a 1 m-deep model river with a 1 m/s current velocity and a 3 m/s wind speed is 5.4 hours (1, 2). Similarly, the volatilization half-life for a 1 m-deep model lake with a 0.05 m/s current and 0.5 m/s wind is 5.1 days (2). The rate of volatilization is controlled by the movement of naphthalene in water, and is therefore much more sensitive to the current velocity than the wind speed. A ten-fold decrease in current to 0.1 m/s will increase the half-life to 32 hours, whereas a ten-fold decrease in wind speed to 0.3 m/s will increase the half-life to 11 hours (1). The rate of evaporation of naphthalene in jet fuel from water relative to the oxygen reaeration rate ranged from 0.2 to 0.5 which, when combined with typical reaeration rates for natural bodies of water (4), gives a half-life for evaporation of 50 hours and 200 hours in a model river and a model lake, respectively (3).

Naphthalene adsorbs moderately strongly to soil and sediment. The mean K_{oc} for 17 soils and sediments was 871 (6) and that for soils from Switzerland was 812 (8). Mean measured K_{oc} values were 2400 for 4 silt loams and a sandy loam soil (7) and 594 (range 420-830) for 5 soils of different clay and organic carbon content (19). A K_{oc} of 4100 was measured for fine natural estuarine colloids (17). Estimated volatilization half-lives from a soil containing 1.25% organic carbon were 1.1 days from a 1 cm soil depth and 14.0 days from a 10 cm soil depth (10). In a variety of surface waters, only 0.1-0.8% of the naphthalene was sorbed to particulate matter (16). The estimated volatilization half-life was increased to 65 hours due to sediment adsorption in a flowing river of 5 m/s and 1 m depth (16).

After a release of petroleum-derived fuels or solvents, nonaqueous phase liquids are retained in the pore space of soils or as a thin film. Naphthalene will partition independently to these liquids and the soil organic carbon. Soils contaminated with residual hydrocarbons, therefore, will adsorb naphthalene to a much greater extent, (nearly 2 orders of magnitude greater in Lincoln sand) than do uncontaminated soil (18).

Partitioning of organic compounds to dissolved organic matter can reduce their *apparent* partitioning to soil and facilitate leaching into soil (20). This explains the appearance of naphthalene in groundwater or in leachate under rapid infiltration sites and in laboratory column leaching experiments and field studies (9-14), despite its moderately strong adsorption to aquifer material (15).

[(1) Southworth GR; Bull Environ Contam Toxicol 21: 507-14 (1979) (2) Lyman WJ et al; Handbook of Chemical Property Estimation Methods Environmental behavior of organic chemicals; New York, NY: McGraw Hill p. 960 (1982) (3) Smith JH, Harper JC; 12th Conf on Environ Toxicol; pp. 336-53 (1982) (4) Mill T et al; Laboratory protocols for evaluating the fate of organic chemicals in air and water; p. 255 EPA-600/3-82-022 (1982) (5) Jury WA et al; J Environ Qual 13: 573-9 (1984) (6) Karickhoff SW; Chemosphere 10: 833-46 (1981) (7) Briggs GG; J Agric Food Chem 29: 1050-9 (1981) (8) Schwarzenbach RP, Westall J; Environ Sci Technol 15: 1360-7 (1981) (9) Goerlitz DF; Bull Environ Contam Toxicol 32: 37-44 (1984) (10) Hutchins SR et al; Environ Toxicol Chem 2: 195-216 (1983) (11) Roberts PV et al; J Water Pollut Control Fed 52: 161-71 (1980) (12) Schwarzenbach RP et al; Environ Sci Technol 17: 472-9 (1983) (13) Piet GJ et al; Int Symp Quality of Groundwater Studies in Environ Sci 17: 557-64 (1981) (14) Rittmann BE et al; Ground Water 18: 236-43 (1980) (15) Ehrlich GG et al; Ground Water 20: 703-10 (1982) (16) Herbes SE et al; pp. 113-28 In: Scientific Basis of Toxicity Assessment; Witschi H ed; Elsevier/North Holland Biomed Press (1980) (17) Wijayaratne RD, Means JC; Mar Environ Res 11: 77-89 (1984) (18) Bouchard DC et al; Chemosphere 21: 975-89 (1990) (19) Kishi H et al; Chemosphere 21: 975-89 (1990) (20) Khan AT, Tomson MB; Environ Toxicol Chem 9: 253-63 (1990) (21) U.S. EPA; PCGEMS (Graphical Exposure Modeling System), PCENPART (Environmental Partitioning Model)]

Persistence: Naphthalene absorbs light with wavelengths greater than 290 nm and may photolyze in surface water and air (1, 3). The photolysis half-life of naphthalene in surface waters is estimated to be 71 hours (1, 2), but will be longer in deeper or murky water (1). When a mixture of jet fuel was added to filtered deionized water, salt water, or pond water and exposed to sunlight, 44-77% of the naphthalene in the fuel was lost in 7 days (6). The presence of algae in water can increase the photolysis rate of naphthalene by a factor of 1.3 to 2.7 (5). Mutagenic photolysis products are formed when nitrite is present in the water (4). Naphthalene does not hydrolyze or react appreciably with oxidizing species in natural waters (3).

In the atmosphere, naphthalene reacts with photochemically-produced hydroxyl radicals with a rate constant of $2.16 \times 10^{-11} \text{ cm}^3/\text{molecule-s}$ (7). Assuming a hydroxyl radical concentration of $5 \times 10^5 \text{ radicals/cm}^3$, the half-life of naphthalene in the atmosphere will be 17.7 hours. Loss due to reaction with ozone and NO_3 radicals will be negligible (8). The average lifetime as a result of reaction with NO_3 , assuming a 12-hour nighttime NO_3 radical concentration of $2.4 \times 10^8 \text{ radicals/cm}^3$ and a NO_2 concentration of $2.4 \times 10^{12} \text{ molecules/cm}^3$ is 100 days. Similarly, the half-life as a result of reaction with ozone at a concentration of $2.4 \times 10^{12} \text{ molecules/cm}^3$ is >80 days (8).

Results of standard biodegradability tests and die-away tests in natural systems indicate that naphthalene biodegrades after a relatively short acclimation period (9). Degradation can be rapid in oil-contaminated water and slow in unpolluted water. The degradation rate increases with naphthalene concentration. For biodegradation to occur, naphthalene must be dissolved in water (10). In die-away tests, reported half-lives include: 3 days in water containing high levels of PAHs (2); 7, 24, 63, and 1,700 days in an oil-polluted estuarine stream, an unpolluted estuarine stream, coastal waters, and the Gulf Stream, respectively (11); and 3 to 9 days in water near a coal-coking wastewater outfall (2, 12). In water from the Alaskan continental shelf, degradation rates average 0.5%/week; however, when nutrient levels are very low, such as after algae blooms in the late spring and early summer, degradation rates are lower (13).

Biodegradation rates of naphthalene in sediment are much greater than in the water column above the sediment, for example, 8- to 20-fold higher, in one experiment (14). Reported half-lives for naphthalene in sediment include: 9 days near a coal-coking discharge (12) and 3, 5, and >2,000 hours in sediment with high, medium, and low levels of PAHs, respectively (2). Biodegradation half-lives range from 2.4 weeks in sediments that were chronically exposed to petroleum hydrocarbons to 4.4 weeks in sediment from clean environments (15).

Naphthalene biodegradation in intertidal sediment is dependent on the availability of oxygen in the sediment (20, 21). No degradation occurs in the absence of oxygen. Naphthalene degraded in aerobic groundwater from a surficial well in Florida, but not in anaerobic groundwater (22). No naphthalene degradation was observed in 6 and 11 weeks in an anaerobic laboratory reactor using seed from a well near a source of contamination (16), or with sewage seed (17), respectively. However naphthalene was completely degraded in 8 days in gas-oil saturated groundwater which was circulated through sand under aerobic conditions (18). The latter case indicates that some species of ubiquitous microflora present in clean groundwater are capable of degrading naphthalene under aerobic conditions. Naphthalene is biodegraded in anoxic soil-water systems under denitrifying conditions. In this case, soil microorganisms are able to degrade naphthalene by utilizing nitrate as an electron acceptor. In experiments with a soil:water ratio of 50:1, naphthalene concentrations were reduced to undetectable levels in 33-47 days, including a 2 week lag period (19).

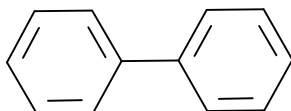
[(1) Zepp RG, Schlotzhauer PF; pp. 141-58 In: Polynuclear Aromatic Hydrocarbons; Jones PW, Leber P ed. Ann Arbor, MI: Ann Arbor Press (1979) (2) Herbes SE et al; pp. 113-28 In: Scientific Basis of Toxicity Assessment; Witachi H ed; Elsevier/North Holland Biomed Press (1980) (3) Callahan MA et al; Water-related environmental fate of 129 priority pollutants; pp. 95-1 to 95-20 EPA-440/4-79-029b (1979) (4) Suzuki J et al; Bull Environ Contam Toxicol 31: 79-84 (1983) (5) Zepp RG, Schlotzhauer PF; Environ Sci Technol 17: 462-8 (1983) (6) Smith JH, Harper JC; 12th Conf on Environ Toxicol; pp. 336-53 (1982) (7) Atkinson R; J Phys Chem Ref Data, Monograph 1 (1989) (8) Atkinson R et al; Lifetimes and fates of toxic air contaminants in California's atmosphere. ARB/R-90/441 p. H-40. California Air Resources Board, Sacramento, CA (1990) (9) Van der Linden AC; Dev Biodegrad Hydrocarbons 1: 165-200 (1978) (10) Thomas JM et al; Appl Environ Microbiol 52: 290-296 (1986) (11) Lee RF; pp. 60-70 In: Fate and Effects of Petroleum Hydrocarbons in Marine Organisms and Ecosystems Volume 6. Wolfe DA ed. (1977) (12) Herbes SE; Appl Environ Microbiol 41: 20-8 (1981) (13) Roubal G, Atlas RM; Appl Environ Microbiol 35: 897-905 (1978) (14) Herbes SE, Schwall LR; Appl Environ Microbiol 35: 306-16 (1978) (15) Heitkamp MA et al; Appl Environ Microbiol 53: 129-36 (1987) (16) Ehrlich GG et al; Ground Water 20: 703-10 (1982) (17) Bouwer EJ, McCarty PL; Appl Environ Microbiol 45: 1295-9 (1983) (18) Kappeler T, Wuhrmann K; Water Res 12: 327-33 (1978) (19) Mihelcic JR, Luthy RG; Appl Environ Microbiol 54: 1188-1198 (1988) (20) Bauer JE, Capone DG; Appl Environ Microbiol 50: 81-90 (1985) (21) DeLaune RD et al; Mar Pollut Bulletin 11: 103-106 (1980) (22) Delfino JJ, Miles; Soil Crop Sci Soc FL Proc 44: 9-14 (1985)]

BIPHENYL

SUBSTANCE IDENTIFICATION

Synonyms: 1,1'-Biphenyl; diphenyl; phenylbenzene

Structure:



CAS Registry Number: 92-52-4

Molecular Formula: C₁₂H₁₀

CHEMICAL AND PHYSICAL PROPERTIES

Boiling Point: 255.2 °C

Melting Point: 69.2 °C

Molecular Weight: 154.21

Dissociation Constants: Not applicable

Log Octanol/Water Partition Coefficient (log K_{ow}): 4.09 (1)

Water Solubility: 7.09 mg/L (2)

Vapor Pressure: 8.93 x 10⁻³ mm Hg @ 25 °C (3)

Henry's Law Constant: 3.00 x 10⁻⁴ atm-m³/mole (4)

Lower Explosive Limit: 0.6% @ 232 °F (5)

[(1) Hansch C, Leo AJ; Medchem Project Issue No 26 Claremont, CA: Pomona College (1985) (2) Pearlman RS et al; J Chem Ref Data 13: 555-562 (1984) (3) Burkhard LP et al; J Chem Eng Data; 29: 248-250 (1984) (4) Mackay D et al; Volatilization of organic pollutants from water EPA-600/53-82-019 (1982) (5) Sax NI; Dangerous Properties of Industrial Materials 5th Edition, p. 622 (1979)]

EXPOSURE PROFILE

Production: The U.S. ITC reports 1991 biphenyl sales of 17.9 million pounds (3). The production volume of biphenyl for 1991 was not disclosed (1). In 1990, there were biphenyl sales of 23.4 million pounds out of a production of 53.5 million pounds (3). Biphenyl is produced by Chemol Co. (Greensboro, NC), Koch Refining (Corpus Christi, TX), Monsanto (Anniston, AL), and Sybron Chemicals (Wellford, SC) (2). Kirk-Other lists the principal producers as Dow, Monsanto, and Koch Refining., with lesser amounts produced by Sybron Chemicals and Chemol Co. (4). Except for Monsanto, biphenyl is produced as a byproduct of the hydrodealkylation (HDA) of toluene to benzene; approximately 1 kg of biphenyl is recovered from the higher boiling residues per 100 kg of benzene produced (4). Approximately half of biphenyl produced in 1990

was derived from HDA sources (4). High purity biphenyl is produced by Monsanto by the direct dehydrocondensation of benzene (4).

Byproduct biphenyl is generally shipped in the molten state by tank car or tank truck. Higher purity grades are either sold in the molten state in tank truck or tank car lots or as flakes in bags or drums (4, 5).

According to the 1991 Toxics Release Inventory, biphenyl is produced at 37 locations and imported by companies in four other locations (see Appendix) (8). Many of these companies are engaged in petroleum refining or steel production and produce biphenyl as an impurity or byproduct. Eight of the facilities indicate that the biphenyl is for sale and/or distribution and 7 indicate that it is for on-site use or processing. Over 10 million pounds of biphenyl may be stored on-site at two locations and over 1 million pounds may be stored on-site at another 8 locations.

[(1) USITC; Synthetic Organic Chemicals. United States Production and Sales, 1991. USITC Publication 2607. pp. 3-2, 3-4. February 1993 (2) SRI International; 1993 Directory of Chemical Producers, United States of America p. 478 (1993) (3) USITC; Synthetic Organic Chemicals. United States Production and Sales, 1990. USITC Publication 2470. pp. 3-2. December 1991 (4) Thompson QE; Kirk-Othmer Encyclopedia of Chemical Technology 4th ed 4: 223-237 (1992) (5) Chemcyclopedia94; p. 73, American Chemical Society, Washington, DC (1994) (6) U.S. EPA; Toxics Release Inventory (1992)]

Use: Biphenyl is used as a heat transfer agent, a dye carrier for polyesters, a feedstock, especially in the production of alkylbiphenyls, and a citrus fruit wrapping impregnate to reduce spoilage (1, 2, 3). One common heat transfer fluid, Dowtherm A, is a eutectic mixture containing 26.5% biphenyl and 73.5% diphenyl ether (2). About 10% of the byproduct biphenyl is consumed as technical grade (93-95%) material as a textile dye carrier and the rest is used as an alkylation feedstock or purified and used as a heat transfer agent (1). High purity biphenyl from the dehydrocondensation of benzene is used as a heat transfer agent or alkylated (1). Alkylated biphenyls are used as heat transfer agents and dielectric fluids in condensers (1). Biphenyl is listed as an important and commonly found food preservative (2). The U.S. FDA lists it as a flavor enhancer or adjuvant (4). The label notation for biphenyl is E230 and the recommended concentration range is 50-70 ppm (2).

The use of biphenyl as a dye carrier in the textile industry has been on the decline because of environmental concerns over the amount of biphenyl released in wastewater effluents by the many plants that dye textiles (1). Biphenyl in these effluents may be converted to polychlorinated biphenyls (PCBs) during chlorination of wastewater.

Formerly, biphenyl was chlorinated to form PCBs for use as a nonflammable hydraulic fluid and transformer dielectric. Production of PCBs ceased precipitously in 1972 when they were recognized as serious environmental contaminants (1).

[(1) Thompson QE; Kirk-Othmer Encyclopedia of Chemical Technology 4th ed 4: 223-237 (1992) (2) Paetz C; Ullmann's Encyclopedia of Industrial Chemistry A13: 261-264 (1989) (3) Chemcyclopedia94; p. 73, American Chemical Society,

Occupational Exposure: NIOSH (NOES Survey 1981-83) has statistically estimated that 20,351 workers are exposed to biphenyl in the United States (1). Workers may be exposed to biphenyl by inhalation and dermal contact in industries that produce biphenyl or use it as a dye carrier (e.g., textile industry), heat transfer material, feedstock, or for impregnating paper. Exposure may be especially high during the loading and unloading of the molten material. Workers involved in wrapping or handling fruit in biphenyl-impregnated paper may be exposed to biphenyl. Biphenyl may be emitted into air as a vapor or adsorbed to carbonaceous material by industrial processes involving the incomplete combustion of organic materials (e.g., coke ovens, foundries) and constitute a source of worker exposure to biphenyl. Limited monitoring data are available for the biphenyl-impregnated paper industry where the potential for exposure is high due to the open nature of the machinery and the elevated temperatures required for the process. Impregnation is usually performed at paper mills and involves dissolving biphenyl in paraffin oil and applying the mixture to paper using a heated roller (7). Reels of paper are distributed to users in the fruit industry. The highest average biphenyl concentration in a paper machine hall of a Finnish impregnating plant was 10.1 ppm, behind the impregnating roller (7). Concentrations were particularly high in the room where measuring and mixing occurred; the average biphenyl concentrations during biphenyl addition to a mixing container and above an open measuring container were 11.8 and 19 ppm, respectively (7).

Workers in the paving, roofing, and steel industries were exposed to biphenyl vapor at concentrations of 0.05-0.69 $\mu\text{g}/\text{m}^3$ (2). Workers at silicon carbide plants were exposed to both vapor and particulate biphenyl at concentrations of 0.07-7.6 $\mu\text{g}/\text{m}^3$ (3). Biphenyl was also detected in the vapor phase at an aluminum production plant (4). Workers involved in the treatment of wood with creosote were also exposed to biphenyl (5). Workers were exposed to Dowtherm A, a mixture of biphenyl and biphenyl ether, in a nylon production plant as indicated by hydroxybiphenyl in their urine (6).

[(1) NIOSH. National Institute for Occupational Safety and Health. National Occupational Exposure Survey (NOES). Computer printout March 29, 1989 (2) Lesage J et al; Am Ind Hyg Assoc J 48: 753-9 (1987) (3) Dufresne A et al; Am Ind Hyg Assoc J 48: 160-6 (1987) (4) Bjorseth A et al; Scand J Work Environ Health 7: 223-32 (1981) (5) Heikkila PR et al; Scand J Work Environ Health 13: 431-7 (1987) (6) Dorgelo FO et al; Int Archives Occupat Environ Health 56: 129-134 (1985) (7) Hakkinen I et al; Arch Environ Health 26: 70-74 (1973)]

Consumer Exposure: Consumer exposure to biphenyl will be from consuming foods containing biphenyl as a food additive and smoking cigarettes. Consumers may also be exposed to biphenyl from the biphenyl-impregnated paper on citrus.

Environmental Release and General Population Exposure: According to the 1991 Toxics Release Inventory (TRI), 956,685 pounds of biphenyl were released to the environment, of which 89.9% was released into the atmosphere, 2.0% into water, 3.2% onto land, and 4.9% injected underground (1). Biphenyl is a minor component of petroleum (3). Biphenyl is a product of the combustion of biomass, coal, diesel oil, gasoline, wood, refuse, and plastics (4, 7, 8). Biphenyl

was the second most abundant product identified by mass spectroscopy in the incineration of polystyrene (5). Biphenyl is one of the major components of creosote and it may be emitted at creosote impregnation facilities and from creosote-treated wood (6). It is also found in cigarette smoke (4).

In a comprehensive survey of wastewater from 4,000 industrial and publicly owned treatment works (POTWs) sponsored by the Effluent Guidelines Division of the U.S. EPA, biphenyl was identified in discharges of the following industrial category (positive occurrences; median concentration in ppb): timber products (13; 1241.6), iron and steel manufacturing (1; 12.2), petroleum refining (3; 13.8), nonferrous metals (1; 42.9), printing and publishing (1; 38.7), ore mining (4; 20.5), coal mining (6; 30.6), organics and plastics (23; 192.8), textile mills (6; 276.4), plastics and synthetics (8; 55.2), pulp and paper (3; 24.5), rubber processing (2; 56.1), soaps and detergents (2; 90.7), auto and other laundries (2; 26.6), pesticides manufacture (1; 81.5), photographic industries (1; 6.8), gum and wood industries (2; 16.6), pharmaceuticals (9; 71.1), foundries (5; 11.3), aluminum (1; 15.0), electroplating (1; 50.6), oil and gas extraction (1; 1.4), organic chemicals (37; 62.7), mechanical products (2; 253.7), transportation equipment (2; 15.9), and POTWs (89; 38.2) (2). Industries (highest concentration effluent in *ppm*) for which the highest effluent concentration was greater than 1 ppm were: organics and plastics (139.1), timber products (55.9), organic chemicals (5.9), pharmaceuticals (2.8), POTWs (1.3) (2). At least 95% of biphenyl used as a dye carrier is released in wastewater (16). Additional biphenyl may volatilize from the dye bath or be removed from the dyed fabric during vacuum drying. Other investigators have found biphenyl in effluents from textile plants at a level of at least 26 µg/L (17, 20), and in water treatment plants (19, 25), coal gasification and natural gas production (21-23), sewage treatment plants (24), and petroleum refineries (26). Biphenyl has also been found in urban runoff (18).

Biphenyl has been detected in both the gas and the particle phase of urban air samples (9, 10). The concentration of biphenyl in air along the Niagara River, NY in 1982-1983 ranged from 0.49 to 96 ng/m³ (11). In 1986, the concentration of biphenyl in ambient air in Torrance, CA was 0.06 µg/m³ (13). The biphenyl concentration in air in Glendora, CA during a smog episode in 1986 ranged from 0.036 to 0.22 µg/m³ (12). Biphenyl was detected in indoor air in Washington, DC and Chicago, IL at concentrations greater than 5 ppb (14). It was also detected in 4 of 8 personal air of subjects from New Jersey and North Carolina (15).

Biphenyl was detected in drinking water in the U.S. (27) and in the U.K. (28). It was detected in drinking water from Ottawa, Canada at 0.7-1.1 ng/L and from Eastern Ontario, Canada at 0.1-1.7 ng/L (29, 30). The concentration of biphenyl in drinking water from 12 Canadian treatment plants ranged from 0.3 to 31.9 ng/L (31). Biphenyl has been measured in the Great Lakes at levels from ND to 4.0 ng/L (32) and the lower Tennessee River, KY at 36.8 µg/L (33, 34). It has also been detected in the Mississippi and Merrimack Rivers (35, 36). Biphenyl has been detected in groundwaters adjacent to a wood-preserving chemical manufacturing facility in Pensacola, FL (37), near an abandoned creosote manufacturing facility at Conroe, TX at levels up to 225 µg/L (38,40), at an underground coal gasification unit in Wyoming at levels of 23-43 µg/L (39),

beneath a coal-tar distillation and wood treatment plan in Minnesota at 12 ng/L (42), and under a coal and oil gasification plant in Seattle, WA at 10-70 µg/L (41). Biphenyl has also been detected in rain in west Los Angeles and Pasadena, CA (43).

The concentration of biphenyl in coastal sandy loam soil in New Jersey that was contaminated with coal tar more than 40 years earlier was 0.9 ppm (44). The soil samples were obtained at a depth of 180 cm below the surface. Biphenyl was also detected in soil beneath a coal tar distilling and wood preserving plant in Minnesota at 0.13-0.3 ppm (45).

Biphenyl was detected in sediment from a small New England river at 1-2 ppm (46). It was also detected in sediments from Puget Sound, WA at 8.5-410 ppb (47) and Rhode Island Sound, RI at 5.5-22.9 ppb (48). The concentration of biphenyl in sediment was 46.9 ppb at a distance of 25 m from an offshore multiwell platform in the Gulf of Mexico and 0.3 ppb at a distance exceeding 25 m from the platform. On the other hand, no biphenyl was detected (detection limit, <5 µg/kg) in sediments from coastal estuarine sites (49).

Biphenyl was found at levels exceeding 70 ppm in Florida grapefruits treated with biphenyl as a fungistat (53). It was qualitatively detected as a residue in foods in the FDA pesticide monitoring program for fiscal years 1978-1982 (54). Biphenyl has been identified as a volatile component of baked potatoes (50), cassava (51), and roasted filberts (52).

In EPA's National Human Adipose Tissue Survey (NHATS) for fiscal year 1982, biphenyl was detected in 9 of 44 composite samples (55). The biphenyl concentration in two of these samples was 1 ppb, and was <1 in the other samples.

[(1) U.S. EPA; Toxics Release Inventory (1992) (2) Shackelford WM et al; *Analyt Chim Acta* 146: 15-27 (supplemental data) (1983) (3) Elliott JJ, Melchior MT; Kirk-Othmer Encyclopedia of Chemical Technology 3rd ed 17: 123-125 (1982) (4) Graedel TE et al (eds); *Atmospheric Chemical Compounds*. p. 184 New York, NY: Academic Press (1986) (5) Hawley-Fedder RA et al; *J Chromatography* 315: 201-210 (1984) (6) Heikkila PR et al; *Scand J Work Environ Health* 13: 431-437 (1987) (7) Wienecke J et al; *Chemosphere* 25: 1889-1895 (1992) (8) Wienecke J et al; *Chemosphere* 25: 437-447 (1992) (9) Cautreels W, Van Cauwenberghe K; *Atmos Environ* 12: 1133-41 (1978) (10) Krstulovic AM et al; *Am Lab* 9: 11-8 (1977) (11) Hoff RM, Chan K; *Environ Sci Technol* 21: 556-61 (1987) (12) Arey J et al; *Atmos Environ* 21: 1437-44 (1987) (13) Atkinson R et al; *Environ Sci Res* 36: 291-309 (1987) (14) Jarke FH et al; *Ashrae Trans* 87: 153-66 (1981) (15) Wallace LA et al; *Environ Res* 35: 293-319 (1984) (16) Meylan WM, Howard PH; Chemical market input/output analysis of selected chemical substances to assess sources of environmental contamination. Task II: Biphenyl and diphenyl oxide. EPA 560/6-77-003. pp. 40-41 (1977) (17) Gordon AW, Gordon M; *Trans Ky Acad Sci* 42: 149-57 (1981) (18) Hoffman EJ et al; *Environ Sci Technol* 18: 580-7 (1984) (19) Gaffney PE; *J Water Pollut Control Fed* 48: 2731-7 (1976) (20) Garrison AW, Hill DW; Organic Pollutants from Mill Persist in Downstream Waters, *Am Dyestuff Reporter*, Feb (1972) (21) Giabbai MF et al; *Int J Environ Anal Chem* 20: 113-29 (1985) (22) Pellizzari ED et al; *ASTM Spec Tech Publ* No. 686 pp. 256-74 (1979) (23) Davani B et al; *Int J Environ Anal Chem* 20: 205-23 (1985) (24) Eganhouse RP, Kaplan IR; *Environ Sci Technol* 16: 541-51 (1982) (25) Hutchins SR et al; *Environ Toxicol Chem* 2: 195-216 (1983) (26) Snider EH, Manning FS; *Environ Int* 7: 237-58 (1982) (27) Kool HJ et al; *Crit Rev Environ Control* 12: 307-57 (1982) (28) Fielding M et al; Organic micropollutants in drinking water. WRC Environmental Protection Tech Report No. 159, Medmenham Lab, Medmenham, UK (1981) (29) Benoit FM et al; *Int J Environ Anal Chem* 6: 277-87 (1979) (30) Benoit FM et al; *Bull Environ Contam Toxicol* 23: 774-8 (1979) (31) Williams D et al; *Chemosphere* 11: 263-76 (1982) (32) Lebel GL et al; *Adv Chem Ser* 214: 309-25 (1987) (33) Goodley PC, Gordon M; *Trans Ky Acad Sci* 37: 11-5 (1976) (34) Gordon M, Goodley PC; *Amer Chem Soc Div Water Air Waste Chem, General Paper* 11: 91-4 (1971) (35) Hites RA; *J Chromatogr Sci* 11: 570-4 (1973) (36) Overton EB et al; *Chemosphere* 9: 629-33 (1980) (37) Goerlitz DF et al; *Environ*

Sci Technol 19: 955-61 (1985) (38) Bedient PB et al; Ground Water 22: 318-29 (1984) (39) Steurmer DH et al; Environ Sci Technol 16: 582-7 (1982) (40) Thomas J et al; J Ind Microbiol 4: 109-20 (1989) (41) Turney GL, Goerlitz DF; Ground Water Monit Rev 10: 187-98 (1990) (42) Ehrlich GG et al; Ground Water 20: 703-10 (1982) (43) Simoneit BRT, Mazurek MA; Aerosol Sci Technol 10: 267-91 (1989) (44) Yu X et al; Environ Sci Technol 24: 1732-1736 (1990) (45) Ehrlich GG et al; Ground Water 20: 703-10 (1982) (46) Jungclaus GA et al; Environ Sci Technol 12: 88-96 (1978) (47) Malins DC et al; Carcinogenesis 6: 1463-9 (1985) (48) Pruell RJ, Quinn JG; Toxicol Environ Chem 10: 183-200 (1985) (49) Brooks JM et al; Environ Sci Technol 24: 1079-85 (1990) (50) Coleman EC et al; J Agric Food Chem 29: 42-8 (1981) (51) Dougan J et al; J Sci Food Agric 34: 874-84 (1983) (52) Kinlin TE et al; J Agric Food Chem 20: 1021-8 (1972) (53) Wardowski WF et al; J Amer Soc Horticul Sci 10: 440-3 (1979) (54) Yess NJ et al; J Assoc Off Anal Chem 74: 265-72 (1991) (55) Onstot JD, Stanley JS; Identification of SARA compounds in adipose tissue. pp. 39, B-3, EPA-560/5-89-003 (1989)]

Environmental Transport and Persistence:

Bioaccumulation: The bioconcentration factors (BCF) for biphenyl in golden orfe (*Leuciscus idus melanotus*) and rainbow trout (*Salmo gairdneri*) are 280 (1) and 437 (2), respectively. A BCF of 340 has been reported for biphenyl for an unspecified fish (3).

[(1) Freitag D; Chemosphere 16: 589-98 (1987) (2) Neely WG et al; Environ Sci Technol 8: 1113-5 (1974) (3) Lyman WJ et al; Handbook of Chemical Property Estimation Methods Environmental Behavior of Organic Chemicals; New York, NY: McGraw Hill p. 5-12 (1982)]

Volatilization/ Adsorption: According to a simple fugacity model, the mass distribution of biphenyl among the environmental compartments at equilibrium will be 0.9986 to air and 0.0014 to water (1). Using the Henry's Law constant, the volatilization half-life for biphenyl in a model river 1 meter depth with a current of 1 m/s and a wind speed of 3 m/s is estimated to be 7.2 hours (2). Using the EXAMS model, which includes various input parameters including the effect of adsorption, the volatilization half-life from a model pond has been estimated to be 20 days (3).

The K_{oc} in three soils ranged from 870 to 3300 (4). The mean K_{oc} in five soils was 1450 (6). These K_{oc} values indicate that biphenyl should have "low" to "slight" mobility in soil (5).

Biphenyl volatilizes rapidly from the soil surface. Significant volatilization losses occurred in dark controls for photodegradation studies in three diverse soils representing climatic regions of the U.S. (7).

[(1) U.S. EPA; PCGEMS (Graphical Exposure Modeling System), PCENPART (Environmental Partitioning Model) (2) Lyman WJ et al; Handbook of Chemical Property Estimation Methods Environmental behavior of organic chemicals; New York, NY: McGraw Hill pp. 15-1 to 15-34 (1982) (3) U.S. EPA; EXAMS II Computer Simulation, U.S. EPA, Athens, GA (1987) (4) Southworth GR, Keller JL; Water Air Soil Pollut 28: 239-48 (1986) (5) Swann RL; Res Rev 85: 17-28 (1983) (6) Kishi H et al; Chemosphere 21: 867-76 (1990) (7) Moore WM et al; Soil phase photodegradation of toxic organics at contaminated disposal sites for soil renovation and groundwater quality protection. pp. 14-15, 21, 23-24, 39-44. USGS Report No. G-1304, Reston, VA. NTIS PB-89-237267, Springfield, VA (1989)]

Persistence: In the atmosphere, biphenyl will react with photochemically-produced hydroxyl radicals with a rate constant of $7.0 \times 10^{-12} \text{ cm}^3/\text{molecule-s}$ (1). Using a hydroxyl radical concentration of $5 \times 10^5 \text{ radicals/cm}^3$, the half-life of biphenyl is 2.3 days. The half-lives for the reaction of biphenyl with ozone and nitrate radicals is >80 days and >20 years, respectively (1).

Biphenyl readily biodegraded in laboratory tests using wastewater and activated sludge inocula (2-6, 14). The biodegradation rate is faster when the inocula are acclimated (6, 14). In a river die-away study using Tittabawassee River (Midland, MI) water, the biodegradation half-life of biphenyl was 2-3 days (7). The biodegradation half-life of biphenyl in clean seawater from Seward, AK was 2.8 months (8). When groundwater from an abandoned creosote manufacturing facility containing 25 mg/L biphenyl was incubated under aerobic conditions, no detectable (detection limit, 3.5 ng/L) biphenyl was found within 3 weeks (9). In another study in which 3.0 mg/L of biphenyl was incubated in contaminated groundwater from the American Creosote Works in Pensacola, FL, biphenyl was undetectable within 5 days (13); however, in this study, the incubation was carried out under aerobic conditions. In an ecocore microcosm study using water/undisturbed sediment, the half-life for the primary biodegradation of biphenyl was 2-3 days; mineralization accounted for 38-42% of total biphenyl loss (11). The presence of oxygen enhances subsurface biphenyl biodegradation (12). Under anaerobic conditions, biphenyl biodegrades very slowly (10).

In soil column studies using Lima silt loam soil, 23.8% of the radiolabeled biphenyl initially present (1 ppm) was mineralized after 450 hours (15). While 8.9% of the ^{14}C leached through the column in this period, this was biphenyl metabolites, rather than biphenyl, itself. In other laboratory experiments, approximately 30% and 40% of biphenyl was mineralized in 450 hours in Edwards muck and Lima silt loam soil, respectively (16). The extent of biphenyl mineralization in Flanagan silt loam soil and Altamont soil was 86% in 98 days (18) and 81% in 24 days (17), respectively. In diesel oil contaminated soil, 36% of the biphenyl (31 ppm) degraded in 2 weeks (20). The lag period before biphenyl biodegradation proceeded was 28-48 days in unpolluted soil and 2.4 days and 0.6-1.8 days in soil slightly and heavily polluted with fuel oil, respectively (19)

[(1) Atkinson R; Lifetimes and fates of toxic air contaminants in California's atmosphere. Statewide Air Pollution Research Center, University of California, Riverside, CA. Report 1990, ARB-R-90/441, pp. H16, H17, H21, H33, H38, H40 (1990) (2) Freitag D; Chemosphere 16: 589-98 (1987) (3) Korte F, Klein W; Ecotoxicol Environ Safety 6: 311-27 (1982) (4) Gaffney PE; J Water Pollut Control Fed 48: 2590-8 (1976) (5) Kitano M; Biodegradation and Bioaccumulation Test on Chemical Substances. OECD Tokyo Meeting. Reference Book ISU-No. 3 pp. 1-37 (1978) (6) Thom NS, Agg AR; Proc R Soc Lond B189: 347-57 (1975) (7) Bailey RE et al; Environ Sci Technol 17: 617-21 (1983) (8) Reichardt PB et al; Environ Sci Technol 15: 75-9 (1981) (9) Thomas JM et al; J Ind Microbiol 4: 109-20 (1989) (10) Pruell RJ, Quinn JG; Toxicol Environ Chem 10: 183-200 (1985) (11) Carson DB et al; pp. 48-59 In: Aquatic Toxicology and Risk Assessment, Volume 13 ASTM STP 1096, Philadelphia, PA (1990) (12) Borden RC et al; Ground Water Monit Rev 9: 83-91 (1989) (13) Mueller JG; Appl Environ Microbiol 57: 1277-1285 (1991) (14) Vaishnav DD, Korthals ET; J Indust Microbiol 8: 209-212 (1991) (15) Aronstein BN, Alexander M; Appl Microbiol Biotechnol 39: 386-390 (1993) (16) Aronstein BN et al; Environ Sci Technol 25: 1728-1731 (1991) (17) Focht DD, Brunner W; Appl Environ Microbiol 50: 1058-63

(1985) (18) Fries GF, Marrow GS; Bull Environ Contam Toxicol 33: 6-12 (1984) (19) Aamand J et al; J Contam Hydrol 4: 299-312 (1989) (20) Wang X et al; Environ Sci Technol 24: 1086-9 (1990)]

APPENDIX

PRODUCERS AND IMPORTERS OF BIPHENYL ACCORDING TO THE 1991 TRI

COMPANY	MANUFACTURE/IMPORT	(SIC CODE) INDUSTRIAL SECTOR	MAXIMUM AMOUNT ON SITE
ASHLAND OIL INC.	Produce As an impurity	(2911) Petroleum refining	100,000-999,999 lbs.
ASHLAND OIL INC.	Produce As an impurity	(2911) Petroleum refining	100,000-999,999 lbs.
ASHLAND OIL INC.	Produce As an impurity	(2911) Petroleum refining	100,000-999,999 lbs.
ATLANTIC RICHFIELD CO.	Produce As an impurity	(2911) Petroleum refining (2869) Industrial organic chemicals (2992) Lubricating oils and greases	1,000,000-9,999,999 lbs.
BETHLEHEM STEEL CORP.	Produce As a byproduct	(3312) Blast furnaces and steel mills	1,000-9,999 lbs.
BETHLEHEM STEEL CORP.	Produce As a byproduct As an impurity	(3312) Blast furnaces and steel mills	10,000-99,999 lbs.
BETHLEHEM STEEL CORP.	Produce As a byproduct	(3312) Blast furnaces and steel mills (3316) Cold finishing of steel shapes (3362) Brass, bronze, copper, copper base alloy foundries	10,000-99,999 lbs.
BF GOODRICH	Produce As an impurity	(2812) Alkalies and chlorine (2821) Plastics materials and resins (2869) Industrial organic chemicals, nec	10,000-99,999 lbs.
CBP RESOURCES INC.	Produce For sale/distribution	(2899) Chemical preparations, nec	10,000-99,999 lbs.
CHEVRON CORP.	Produce For sale/distribution As a byproduct	(2911) Petroleum refining	1,000,000-9,999,999 lbs.
CHEVRON CORP.	Produce For on-site use As a byproduct	(2869) Industrial organic chemicals, nec (2821) Plastics materials and resins (2895) Carbon black	100,000-999,999 lbs.
DOW CHEMICAL CO.	Produce For sale/distribution	(28) Chemicals and Allied Products (2819) Industrial inorganic chemicals, nec (2821) Plastics materials and resins (2834) Pharmaceutical preparations (2869) Industrial organic chemicals, nec (2879) Agricultural chemicals, nec	1,000,000-9,999,999 lbs.
DOW CHEMICAL CO.	Produce As a byproduct As an impurity	(2812) Alkalies and chlorine (2813) Industrial gases (2819) Industrial inorganic chemicals, nec (2821) Plastics materials and resins (2822) Synthetic rubber (2865) Cyclic crudes and intermediates	100-999 lbs.
DOW CHEMICAL CO.	Produce For sale/distribution As a byproduct	(2812) Alkalies and chlorine (2821) Plastics materials and resins (2869) Industrial organic chemicals, nec	1,000,000-9,999,999 lbs.
DOW CORNING CORP.	Produce As a byproduct	(2869) Industrial organic chemicals, nec (2822) Synthetic rubber (2821) Plastics materials and resins	10,000-99,999 lbs.
E. I. DU PONT DE NEMOURS & CO. INC.	Import For on-site use/processing	(2911) Petroleum refining	1,000,000-9,999,999 lbs.
EXXON CORP.	Produce As an impurity	(2869) Industrial organic chemicals, nec (2865) Cyclic crudes and intermediates (2822) Synthetic rubber	1,000,000-9,999,999 lbs.
ICI AMERICAN HOLDINGS INC.	Produce As an impurity	(2869) Industrial organic chemicals, nec	1,000-9,999 lbs.

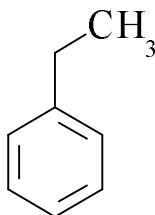
COMPANY	MANUFACTURE/IMPORT	(SIC CODE) INDUSTRIAL SECTOR	MAXIMUM AMOUNT ON SITE
INLAND STEEL INDUSTRIES	Produce As a byproduct	(3312) Blast furnaces and steel mills (3274) Lime	10,000-99,999 lbs.
KALAMA CHEMICAL INC.	Produce As an impurity	(2865) Cyclic crudes and intermediates (2869) Industrial organic chemicals, nec	10,000-99,999 lbs.
KOCH REFINING CO.	Produce For sale/distribution	(2911) Petroleum refining	1,000,000-9,999,999 lbs.
KOCH REFINING CO.	Produce For sale/distribution As a byproduct	(2911) Petroleum refining	10,000,000-49,999,999 lbs.
KOPPERS INDUSTRIES INC.	Produce As an impurity	(2865) Cyclic crudes and intermediates	10,000-99,999 lbs.
KOPPERS INDUSTRIES INC.	Import As an impurity	(2865) Cyclic crudes and intermediates	100,000-999,999 lbs.
KOPPERS INDUSTRIES INC.	Produce As an impurity	(2865) Cyclic crudes and intermediates	10,000-99,999 lbs.
KOPPERS INDUSTRIES INC.	Produce As an impurity	(2865) Cyclic crudes and intermediates	100,000-999,999 lbs.
LTV STEEL CO. INC.	Produce As a byproduct	(3312) Blast furnaces and steel mills (3313) Electrometallurgical products (3316) Cold finishing of steel shapes	100-999 lbs.
LTV STEEL CO. INC.	Produce As a byproduct	(3312) Blast furnaces and steel mills	10,000-99,999 lbs.
LTV STEEL CO. INC.	Produce As a byproduct	(3312) Blast furnaces and steel mills (3313) Electrometallurgical products (3316) Cold finishing of steel shapes	100-999 lbs.
LTV STEEL CO. INC.	Produce As a byproduct	(3312) Blast furnaces and steel mills	100-999 lbs.
MONSANTO CO.	Import For on-site use/processing	(2869) Industrial organic chemicals, nec (2819) Industrial inorganic chemicals, nec (2841) Soap and other detergents (2879) Agricultural chemicals, nec	100,000-999,999 lbs.
MONSANTO CO.	Produce For on-site use/processing For sale/distribution	(2869) Industrial organic chemicals, nec (2865) Cyclic crudes and intermediates	1,000,000-9,999,999 lbs.
NEVILLE CHEMICAL CO.	Produce As a byproduct	(2821) Plastics materials and resins (2869) Industrial organic chemicals, nec	100,000-999,999 lbs.
OCCIDENTAL PETROLEUM CORP.	Produce For on-site use/processing As a byproduct	(2869) Industrial organic chemicals, nec	10,000-99,999 lbs.
PHILLIPS PETROLEUM CO.	Produce For on-site use/processing As a byproduct	(2911) Petroleum refining	10,000,000-49,999,999 lbs.
PIEDMONT CHEMICAL INDUSTRIES INC.	Import For on-site use/processing	(2841) Soap and other detergents	1,000-9,999 lbs.
SUN CO. INC.	Produce As an impurity	(2911) Petroleum refining	1,000-9,999 lbs.
UNION CARBIDE CORP.	Produce As a byproduct	(2869) Industrial organic chemicals, nec	10,000-99,999 lbs.
UNION CARBIDE CORP.	Produce As a byproduct	(2821) Plastics materials and resins (2869) Industrial organic chemicals, nec	100,000-999,999 lbs.
VIRKLER CO.	Produce For sale/distribution	(2869) Industrial organic chemicals, nec (2841) Soap and other detergents (2843) Surface active agents	NO DATA
WEHADKEE YARN MILLS	Import For on-site use/processing	(2269) Finishing plants, nec	0-99 lbs.

ETHYLBENZENE

SUBSTANCE IDENTIFICATION

Synonyms: EB; phenylethane

Structure:



CAS Registry Number: 100-41-4

Molecular Formula: C₈H₁₀

CHEMICAL AND PHYSICAL PROPERTIES

Boiling Point: 136.2 °C

Melting Point: -94.97 °C

Molecular Weight: 106.16

Dissociation Constants: Not applicable

Log Octanol/Water Partition Coefficient (log K_{ow}): 3.15 (1)

Water Solubility: 161 mg/L @ 25 °C (2)

Vapor Pressure: 9.53 @ 25 °C (3)

Henry's Law Constant: 8.44 x 10⁻³ atm-m³/mole (4)

Lower Explosive Limit: 1.2% @ 25 °C (5)

[(1) Hansch C, Leo AJ; Medchem Project Issue No 26 Claremont, CA: Pomona College (1985) (2) Sutton C, Calder JA; J Chem Eng Data 20: 320-322 (1975) (3) Boublik T et al; The Vapor Pressures of Pure Substances. p. 617. Amsterdam: Elsevier (1984) (4) Mackay D et al; Environ Sci Tech 13: 333-6 (1979) (5) Sax NI; Dangerous Properties of Industrial Materials 6th Edition p. 1322 (1984)]

EXPOSURE PROFILE

Production: Ethylbenzene had a 1992 production volume of 11,450 million pounds of which 196 million pounds were exported; an additional 7 million pounds were imported (1). The U.S. ITC reports ethylbenzene sales of 352 million pounds for 1991, out of a production of 8,852 million pounds (2). Ethylbenzene is produced by Cos-Mar (Carville, LA), Arco (Channelview, TX), Sterling (Texas City, TX), Chevron (St. James, LA), Dow (Freeport, TX), Huntsman (Bayport,

TX), Amoco (Texas City, TX), Westlake (Lake Charles, LA), Rexene (Odessa, TX), and Koch (Corpus Christi, TX) (1).

[(1) Chemical Marketing Reporter; Chemical Profile: Ethylbenzene. July 13, 1992 (2) USITC; Synthetic Organic Chemicals. United States Production and Sales, 1991. USITC Publication 2607. p. 3-2 February 1993]

Use: Over 99% of ethylbenzene is used captively in the manufacture of styrene, which is used to produce polystyrene and other plastics (1, 2). The remainder is used as a solvent in the paint industry (1, 2). Minor amounts of ethylbenzene are used in the production of acetophenone, diethylbenzene, and ethyl anthraquinone (2). Ethylbenzene is a component of gasoline (3).

[(1) Chemical Marketing Reporter; Chemical Profile: Ethylbenzene. July 13, 1992 (2) Coty RR et al; Ullmann's Encyclopedia of Industrial Chemistry A10: 35-43 (1987) (3) American Petroleum Institute; Gasoline vapor exposure assessment at service stations. API Publication 4553, pp. 1-21 and Table D-1, page 13 of 15, July 1991 (1993)]

Occupational Exposure: NIOSH (NOES Survey 1981-83) has statistically estimated that 80,726 workers are exposed to ethylbenzene in the United States (1). Workers were exposed to time weighted average (TWA) exposures of 1.2 ppm (5.3 mg/m³) of ethylbenzene during spray painting in paint booths (2). The highest TWA exposure was 4.4 ppm (19 mg/m³) (2). TWA exposure levels of pressroom and plate maker workers ranged from 0.00 to 36 mg/m³ (3). Exposure of roofers to ethylbenzene in adhesive solvents ranged from undetectable to 1.3 mg/m³ (4). Air concentrations of ethylbenzene in 11 paint shops in Spain ranged from 0.5 to 125.0 mg/m³, with a median of 21.8 mg/m³ (5). Maximum TWA air concentrations of ethylbenzene in 10 screen printing plants in The Netherlands ranged from 0.11 to 3.21 mg/m³ (6). The mean and maximum exposures to ethylbenzene while loading a top loading gasoline tank truck are 0.42 ppm and 2.2 ppm (1.8 and 9.7 mg/m³) (9). The concentration of ethylbenzene at one location in an office building with health and comfort complaints ranged from 2.9 to 10 µg/m³, whereas the concentration outdoors ranged from not detectable to 0.9 µg/m³ (7). The average ethylbenzene concentration in three offices of a new office building, before occupancy, was 90 µg/m³; this value dropped to 9 µg/m³ after occupancy (8).

[(1) NIOSH. National Institute for Occupational Safety and Health. National Occupational Exposure Survey (NOES). Computer printout March 29, 1989 (2) Whitehead LW et al; Am Ind Hyg Assoc J 45: 767-72 (1984) (3) Ahrenholz SH; Health Hazard Evaluation Determination Report No. HHE-80-18-691, Looart Press Incorporated, Colorado Spring, Colorado. Hazard Evaluations and Technical Assistance Branch, NIOSH, Cincinnati, Ohio (1980) (4) Reed L; Health Hazard Evaluation Report No. HETA-83-380-1671, Roofing Sites, Dayton, Ohio Hazard Evaluations and Technical Assistance Branch, NIOSH, Cincinnati, Ohio (1986) (5) Medinilla J. Espigares M; Ann Occup Hyg 32: 509-513 (1988) (6) Verhoeff AP et al; Int Arch Occup Environ Health 60: 201-209 (1988) (7) Weschler CJ et al; Am Ind Hyg Assoc J 51: 261-268 (1990) (8) Wallace L et al; Atmos Environ 21: 385-393 (1987) (9) Kawai T et al; Bull Environ Contam Toxicol 46: 1-8 (1991)]

Consumer Exposure: Ethylbenzene was found in 157 of 658 household products surveyed from 65 product categories representing 8 product classes in a study of indoor air pollution chemicals (1, 4). Product *classes* likely to contain ethylbenzene (% of product class) are: paint-related products (47.8%), fabric and leather treatments (11.8%), automotive products (7.5%), cleaners for electronic equipment (4.5%), and household cleaners and polishers (1.2%) (4). The mean

concentrations of ethylbenzene in product classes *for products containing ethylbenzene* are automotive products (7.2%), paint-related products (2.4%), and fabric and leather treatment (1.0%) (4). Product *categories* that are likely to contain ethylbenzene are: spray paint, primers, paint removers, paint thinners, wood stains, varnishes, and finishes, carburetor and choke cleaners, spot removers, water repellent, wood cleaner, tape recorder cleaners, tire cleaner, and paint (1). For spray paints and primers, 64% and 68% of the respective products in the product category contained ethylbenzene. This high occurrence of ethylbenzene in household products indicates that there is a high potential for consumer exposure to ethylbenzene. For example, 85 of the 132 products in the spray paint category contained ethylbenzene (1). According to a national usage survey (2), 35% of households use spray paint. Assuming equal use of spray paint containing ethylbenzene and those that do not contain ethylbenzene, 23% of households in the U.S., approximately 21 million households or 55 million consumers (3) are exposed to ethylbenzene from spray paint. Cleaning a car engine increases exposure to ethylbenzene (4). In a study of customer exposure to gasoline components at 6 service stations in 3 geographical locations, the air concentrations of ethylbenzene at these stations (12 samples) were all 0.1 ppm, while ethylbenzene samples taken at the perimeter of the stations were all 0.005 ppm (5).

[(1) Sack TM, Steele DH; Indoor air pollutants from household product sources. U.S. EPA: Environmental Monitoring Systems Laboratory. EPA/600/S4-91/025 (1992) pp. 1-4, 19, 29-30 (2) Westat, Inc; Household solvent products: A national usage survey. EPA-OTS 560/5-87-005 pp. 1vii - 1xvii (1987) (3) U.S. Department of Commerce; Statistical Abstract of the United States 1988, 108th ed p. 43, 46 (1987) (4) Sack TM et al; Atmos Environ 26: 1063-1070 (1992) (4) Wallace LA; Environ Res 50: 37-55 (1989) (5) American Petroleum Institute; Gasoline vapor exposure assessment at service stations. API Publication 4553, pp. 1-21 and Table D-1, page 13 of 15, July 1991 (1993)]

Environmental Release and General Population Exposure: According to the 1991 Toxics Release Inventory (TRI), 8.8 million pounds of ethylbenzene were released to the environment, 98% of which was released into the atmosphere and 0.6% to land (1).

The median concentration of ethylbenzene in air in the U.S. (25 locations, 861 measurements) was 1.1 ppb; the maximum value was 3.3 ppm (2). The average level of ethylbenzene in air in 15 U.S. cities studied in 1979-1984 was 0.6 - 4.6 ppb; the maximum concentration was 31.5 ppb (3). Ethylbenzene concentrations in major western U.S. cities ranged from 0.1 to 27.7 ppb (4, 6-9), with a mean of 2.68 ppb. Representative centers in New Jersey had average ethylbenzene levels ranging from 0.17 to 0.33 ppb (5). Mean values of ethylbenzene in air in two New Jersey cities and Los Angeles/ Contra Costa, CA are 3.2-4.0 $\mu\text{g}/\text{m}^3$ and 0.9-9.7 $\mu\text{g}/\text{m}^3$, respectively; mean personal air samples from the residents were 9.2-19 $\mu\text{g}/\text{m}^3$ and 3.7-11 $\mu\text{g}/\text{m}^3$, respectively (32). Exposure to solvents, especially those used in refinishing furniture, dyes, petroleum, and smoking increased exposure levels (32). Of 36 Chicago metropolitan area homes tested, 57% had detectable levels of ethylbenzene (10). Average concentrations of ethylbenzene in a school and two homes for the elderly were 3.7, 3.6, and 5.5 $\mu\text{g}/\text{m}^3$, respectively (34). Products that emit ethylbenzene and therefore may contribute to indoor exposure are steel wool soap pads, carpet glue, insecticide (solid), and rodenticide (solid) (33).

Ethylbenzene has been found in U.S. municipal water supplies (11-17). Where reported, levels range up to 4 ppb (11, 16, 17). In the 1982 U.S. Ground Water Supply Survey (466 random

samples), 0.6% of samples had ethylbenzene levels above 0.5 ppb (11). The highest concentration of ethylbenzene was 1.1 ppb (11).

Ethylbenzene is found in some surface waters, particularly where there is anthropogenic influence (17-24). Of the 1,101 surface waters analyzed in the U.S. EPA STORET database, 10% had detectable concentrations of ethylbenzene (20). In a survey of 14 heavily industrialized river basins in the U.S., 5 of 210 sites had detectable levels of ethylbenzene; these were in the Chicago area and Illinois River basin (18). Maximum levels reported were 4 ppb for freshwater (18) and 22 ppb for seawater (22). Of the 350 sediment samples analyzed in the U.S. EPA STORET database, 11% had detectable concentrations of ethylbenzene (20). The median concentration was 5 ppm, dry weight (20). Sediment in the lower Tennessee River contained 4 ppb of ethylbenzene (22).

The general population is exposed to ethylbenzene in gasoline and diesel fuel and exhaust (29), cigarette smoke (29), and some food (30, 31).

Ethylbenzene was detected, but not quantified, in 8 of 8 samples of mother's milk analyzed from 4 U.S. urban areas (25). Of the 387 samples of expired air from 54 normal, healthy, urban volunteers, 16.5% were positive; the mean concentration was 1.8 ng/L (26). Ethylbenzene levels in whole blood from 250 subjects ranged from not detected to 59 ppb, with a mean of 1.0 ppb (27). In the U.S. National Human Adipose Tissue Survey (46 composite samples), 96% of the samples were positive (>2 ppb, wet tissue concentration), with a maximum value of 280 ppb (28).

[(1) U.S. EPA; Toxics Release Inventory (1992) (2) Brodzinsky R, Singh HB; Volatile Organic Chemicals in the Atmosphere: An Assessment of Available Data. p. 177. SRI Contract 68-02-3452 (1982) (3) Singh HB et al; Atmos Environ 19: 1911-9 (1985) (4) Arnts RR, Meeks SA; Biogenic hydrocarbon contribution to the ambient air of selected areas EPA 600/3-80-023 (1980) (5) Harkov R et al; J Air Pollut Control Assoc 33: 1177-83 (1983) (6) Altshuller AP et al; Environ Sci Technol 5: 1009-16 (1971) (7) Lonneman WA et al; Environ Sci Technol 2: 1017-20 (1968) (8) Singh HB et al; Atmos Environ 15: 601-12 (1981) (9) Singh HB et al; Atmospheric measurements of selected toxic organic chemicals EPA 600/3-80-072 (1980) (10) Jarke FH et al; ASHRAE Trans 87: 153-66 (1981) (11) Cotruvo JA; Sci Total Environ 47: 7-26 (1985) (12) NAS; The Alkylbenzenes p. III-13 Contract 68-01-4655 (1980) (13) Shackelford WM, Keith, LH; Frequency of organic compounds in surface waters. EPA 600/4-76-062. pp. 68-69 (1976) (14) Bedding ND et al; Sci Total Environ 25: 143-67 (1982) (15) Keith, LH et al; pp. 329-73 In: Identification and Analysis of Organic Pollutants in Water. Keith LH ed (1976) (16) Kleopfer RD, Fairless BJ; Environ Sci Technol 6: 1036-7 (1972) (17) Konasewich D et al; Status report on organic and heavy metal contaminants in the Lakes Erie, Michigan, Huron and Superior Basins. Great Lakes Quality Review Board (1978) (18) Ewing BB et al; Monitoring to detect previously unrecognized pollutants in surface waters EPA 560/6-77-015 (appendix EPA 560/6-77-015a) (1977) (19) Goodley PG, Gordon M; Kentucky Acad Sci 37: 11-5 (1976) (20) Staples CA et al; Environ Toxicol Chem 4: 139-42 (1985) (21) Sauer TC Jr et al; Mar Chem 7: 1-16 (1978) (22) Gschwend PM et al; Environ Sci Technol 16: 31-8 (1982) (23) Sauer TC Jr; Org Geochem 3: 91-101 (1981) (24) Mantoura RFC; Environ Sci Technol 16: 38-45 (1982) (25) Pellizzari ED et al; Bull Environ Contam Toxicol 28: 322-8 (1982) (26) Krotoszynski BK et al; J Anal Toxicol 3: 225-34 (1979) (27) Antoine SR et al; Bull Environ Contam Toxicol 36: 364-71 (1986) (28) Stanley JS; Broad scan analysis of the FY82 national human adipose tissue survey specimens Volume. I Executive Summary p. 5 EPA-560/5-86-035 (1986) (29) Fishbein L; Sci Tot Environ 44: 269-287 (1985) (30) Dumont JP, Adda J; J Agric Food Chem 26: 364-7 (1978) (31) Lovegren NV et al; J Agric Food Chem 27: 851-3 (1979) (32) Wallace L; Toxicol Environ Chem 12: 215-236 (1986) (33) Wallace L et al; Atmos Environ 21: 385-393 (1987) (34) Sheldon L et al; Indoor air quality in public buildings. Volume I. EPA/600/6-88/009a. pp. 202-204. Research Triangle Park, NC: EPA, Environmental Monitoring Systems Lab. (1988)]

Environmental Transport and Persistence:

Bioaccumulation: The BCF values of ethylbenzene in goldfish and clams are 79 (3) and 5 (1), respectively. Using the octanol/water partition coefficient and a recommended regression equation, a BCF value of 140 can be estimated (2). Therefore, it is unlikely that ethylbenzene will bioconcentrate appreciably in aquatic organisms.

[(1) Nunes P, Benville PE Jr; Bull Environ Contam Toxicol 21: 719-26 (1979) (2) Lyman WJ et al; Handbook of Chemical Property Estimation Methods. Environmental Behavior of Organic Compounds Washington, DC: American Chemical Society pp. 5-5 (Eqn 5-2) (1990) (3) Ogata M et al; Bull Environ Contam Toxicol 33: 561-7 (1984)]

Volatilization/ Adsorption: According to a simple fugacity model, the mass distributions of ethylbenzene among the environmental compartments are 0.9975 in air, 0.0024 in water, and 0.0001 in soil (1). Using the Henry's Law constant, the volatilization half-life of ethylbenzene in a model river 1 m deep with a 1 m/s current and a 3 m/s wind can be estimated to be 3.1 hours (2). Similarly, the volatilization half-life from a model lake 1 m deep with a 0.05 m/s current and 0.5 m/s wind is 4.1 days (2). In a mesocosm experiment using conditions simulating Narragansett Bay, MA, the half-life of ethylbenzene was 13 days in winter; evaporation was the primarily loss mechanism (3). Ethylbenzene has a moderate adsorption coefficient according to its measured K_{oc} in silt loam of 164 (4). From its octanol/water partition coefficient, a K_{oc} of 870 can be calculated using a recommended regression equation (2). Ethylbenzene's presence in bank infiltrated water indicates that it can leach through soil (5). Its high vapor pressure and Henry's Law constant and moderate adsorptivity to soil suggests that volatilization from soil will be important for ethylbenzene.

[(1) U.S. EPA; PCGEMS (Graphical Exposure Modeling System), PCENPART (Environmental Partitioning Model) (2) Lyman WJ et al; Handbook of Chemical Property Estimation Methods. Environmental Behavior of Organic Compounds pp. 4-9 (Eqn 4-10), 15-1 to 15-34 Washington, DC: American Chemical Society (1990) (3) Wakeham SG et al; Environ Sci Technol 17: 611-7 (1983) (4) Chiou CT et al; Environ Sci Technol 17: 227-31 (1983) (5) Piet GJ, Morra CF; pp. 31-42 In: Artificial Groundwater Recharge; Hessman L, Olsthorpe TN, ed (1983)]

Persistence: Ethylbenzene reacts with photochemically-produced hydroxyl radicals in the atmosphere with a rate of $7.1 \times 10^{-12} \text{ cm}^3/\text{molecule-s}$ (1). Assuming a hydroxyl radical concentration of $5 \times 10^5 \text{ radicals/cm}^3$, the half life of ethylbenzene in the atmosphere is 2.3 days. After a period of adaptation, ethylbenzene is biodegraded fairly rapidly by sewage or activated sludge (2, 3, 8, 9). It was completely degraded in groundwater in 8 days (4) and in seawater in 10 days (5). Part of the decrease in ethylbenzene concentration from a leaky gasoline storage tank in the Chalk aquifer in England has been attributed to biodegradation (7). In a mesocosm experiment using simulated Narragansett Bay conditions, complete biodegradation occurred in approximately 2 days after a 2 week lag in spring and a 2 day lag in summer (6).

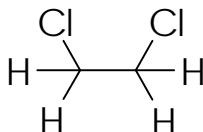
[(1) Atkinson R; J Phys Chem Ref Data. Monograph 1 p. 227 (1989) (2) Tabak HH et al; J Water Pollut Control Fed 53: 1503-18 (1981) (3) Malaney GW, McKinney RE; Water Sewage Works 113: 302-9 (1966) (4) Kappeler T, Wuhrmann K; Water Res 12: 327-33 (1978) (5) Van der Linden AC; Dev Biodegrad Hydrocarbons 1: 165-200 (1978) (6) Wakeham SG et al; Environ Sci Technol 17: 611-7 (1983) (7) Tester DJ, Harker RJ; Water Pollut Control 80: 614-31 (1981) (8) Slave T et al; Rev Chim 25: 666-70 (1974) (9) EPA; Treatability Manual pp. 1.9.8-1 to 1.9.8-5 EPA 600/2-82-001a (1981)]

1,2-DICHLOROETHANE

SUBSTANCE IDENTIFICATION

Synonyms: Ethylene dichloride; DCE

Structure:



CAS Registry Number: 107-06-2

Molecular Formula: C₂H₄Cl₂

CHEMICAL AND PHYSICAL PROPERTIES

Boiling Point: 83.5

Melting Point: -35.7

Molecular Weight: 98.96

Dissociation Constants: not applicable

Log Octanol/Water Partition Coefficient (log K_{ow}): 1.48 (1)

Water Solubility: 8524 mg/L @ 20 °C (2)

Vapor Pressure: 78.9 mm Hg @ 25 °C (3)

Henry's Law Constant: 1.18X10⁻³ atm m³/mole (4)

Lower Explosive Limit: Not available

[(1) Hansch C, Leo AJ; Medchem Project Issue No 26 Claremont, CA: Pomona College (1985) (2) Horvath AL; Halogenated Hydrocarbons: Solubility-Miscibility With Water NY: Marcel Dekker (1982) (3) Daubert TE, Danner RP; Physical & Thermodynamic Properties of Pure Chemicals Vol 1 New York, NY: Hemisphere Pub Corp (1985) (4) Leighton DJJR, Calo JM; J Chem Eng 26: 382-5 (1981)]

EXPOSURE PROFILE

Production: In 1992, the U.S. demand for DCE stood at 14.3 billion pounds, of which 1.4 billion pounds were exported (1). Current U.S. capacity stands at just over 20 billion pounds (1, 2). DCE producers include Borden Chemicals and Plastics (Geismar, LA), Dow Chemical (Freeport and Oyster Creek, TX, and Plaquemine, LA), Formosa Plastics (Baton Rouge, LA, and Point Comfort, TX), Georgia Gulf (Plaquemine, LA), BF Goodrich (La Porte, TX), OxyChem (Convent, LA, and Deer Park and Corpus Christi, TX), Oxymer, (Ingleside, TX), PPG (Lake Charles, LA), Vista (Lake Charles, LA), Vulcan (Geismar, LA), and Westlake (Calvert City, KY) (1, 2).

[(1) Chemical Marketing Reporter; Chemical Profile: Ethylene Dichloride. p. 42, May 11, 1992 (2) SRI International; 1993 Directory of Chemical Producers, United States of America p. 598 (1993)]

Use: The majority of DCE production (88%) is used in the synthesis of vinyl chloride monomer (1). Of the remainder, 10% is exported and 2% is used in a variety of applications including the synthesis of ethylenediamines and other chlorinated solvents (such as 1,1,1-trichloroethane, trichloroethylene, and tetrachloroethylene) (1, 2). Only a small amount of DCE is used as a solvent for dewaxing, deparaffinizing petroleum fractions, in paint, varnish, finish removers, soaps, scouring compounds, wetting and penetrating agents, coating removers, and pesticides, and as a lead scavenger in leaded gasoline (2-3).

[(1) Chemical Marketing Reporter; Chemical Profile: Ethylene Dichloride. p. 42, May 11, 1992 (2) Rossberg, M et al; Ullmann's Encyclopedia of Industrial Chemistry A6: 263-271 (1986) (3) Hawley CG; The Condensed Chemical Dictionary 11th ed. p. 487 New York, NY: Van Nostrand Reinhold Co (1987)]

Occupational Exposure: NIOSH (NOES Survey 1981-1983) has statistically estimated that 77,111 workers are exposed to DCE in the United States (1). Occupational exposure to DCE may occur during its manufacture, formulation, use, and transport. In office buildings, occupational exposure to DCE may also occur by inhalation due to its presence in cleaning agents and construction materials, with a higher potential for exposure in those that are new or newly renovated (2). The concentration of DCE in a newly constructed office building in Research Triangle Park, July to December, 1983, ranged from 5 to 50 ppb (2).

[(1) National Institute for Occupational Safety and Health (NIOSH) National Occupational Exposure Survey (NOES). Computer printout March 29, 1989 (2) Sheldon LS et al; Indoor air quality in public buildings Vol I. pp. 161-172 EPA 600 6-88 009a. PB89-102503 (1988)]

Consumer Exposure: Consumer exposure to DCE may occur by inhalation as a result of volatilization from commercial products in which it is contained. It has been detected in household cleaning agents, pesticide formulations, glued wallpaper, glued carpet products, carburetor and choke cleaners, silicone spray lubricants, paper correction fluid thinner, and rubber repair kits (1-3). Indoor concentrations of DCE have been measured to be as high, or higher, than outdoor concentration obtained concurrently (4, 5).

[(1) Sack TM, Steel DH; Indoor air pollutants from household sources: Project Report. PB92-136837 (1991) (2) EPA; Compilation and speciation of national emissions factors for consumer/commercial solvent use. Information compiled to support urban air toxics assessment studies PB89-207203 (1989) (3) Wallace LA et al; Atmos Environ 21: 385-93 (1987) (4) Pellizzari ED et al; Environ Internatl 12: 619-23 (1986) (5) Sheldon LS et al; Indoor air quality in public buildings Vol I. pp. 161-172 EPA 600 6-88 009a. PB89-102503 (1988)]

Environmental Release and General Population Exposure: According to the 1991 Toxics Release Inventory (TRI), 4 million pounds of DCE were released to the environment, of which 99% was released into the atmosphere, 0.6% to water, 0.15% to underground injection, and 0.17% to land (1). Atmospheric emissions of DCE have also been associated with wastewater sludge incinerators (2) and volatilization from hazardous waste sites (3, 4). Release of DCE to surface water may occur in industrial and wastewater treatment plant effluent (5-8). DCE may

enter ground water as a result of industrial activity as it was detected in on- and off-site wells near a plant producing non-lubricating automotive fluids 8 years after production had ceased (9).

General population exposure to DCE may occur through inhalation as it has been detected in ambient air samples in urban and source dominated areas at median concentrations of 0.012 and 0.26 ppb, respectively (10). A study that compared the indoor and outdoor concentration of volatile organics found DCE was detected in 30% of the indoor and 37% of the outdoor samples (1980, median concentration 0.005 ppb for both) in Greensboro, NC, 89% of the indoor and 100% of the outdoor samples (1981, median concentration 0.60 and 0.44 ppb, respectively) in Baton Rouge, LA, 18% of the indoor and 40% of the outdoor samples (1981, median concentration 0.008 and 0.009 ppb, respectively) in Houston, TX, 64% of the indoor and 44% of the outdoor samples (1984, median concentration 0.044 and 0.042 ppb, respectively) in Los Angeles, CA, and 20% of the indoor and none of the outdoor samples (1984, median concentration 0.08 ppb) in Antioch/Pittsburgh, PA (11).

The presence of DCE in drinking water supplies (12-16) and ground water supplies (17, 18) may also lead to general population exposure through the ingestion of contaminated water. If present in tap water, inhalation exposure to DCE may occur due to its volatilization from water during showers and baths (19). General population exposure to DCE may also occur by ingestion of contaminated food, as it has been detected in grains, milled grain, cereal products, spices, chickpeas, and nectarines (5, 20-24).

[(1) EPA; Toxics Release Inventory (1992) (2) Vancil MA et al; Emissions of metals and organics from municipal wastewater sludge incinerators: Project Summary. EPA/600/S2-91/007 (1991) (3) Barkley J et al; Biomed Mass Spectrom 7: 139-47 (1980) (4) LaRegina J et al; Environ Prog 5: 18-27 (1986) (5) Konietzko H; Chlorinated Ethanes, Sources, Distribution, Environmental Impact, and Health Effects in Hazard Assessment of Chemicals: Current Developments. Academic Press: 3: 401-48 (1984) (6) Bell J et al; Water Environ Res 65: 708-16 (1993) (7) Wilson SC et al; Environ Sci Technol 28: 259-66 (1994) (8) Michael LC et al; Environ Sci Technol 25: 150-55 (1991) (9) US EPA; Superfund Record of Decision, U.S. Aviax, MI PB89-225502 (1988) (10) Shah JJ, Heyerdahl EK; National Ambient VOC Database Update EPA 600/3-88/010 (1988) (11) Pellizzari ED et al; Environ Internatl 12: 619-23 (1986) (12) Coniglio WA et al; Occurrence of volatile organics in drinking water. EPA exposure assessment project draft (1980) (13) Drury JS, Hammons AS; Investigation of selected environmental pollutants: 1,2-Dichloroethanes. EPA-560/78-006 p. 63 (1979) (14) Clark RM et al; Sci Total Environ 53: 153-72 (1986) (15) Suffet IH et al; Water Res 14: 853-67 (1980) (16) EPA; Preliminary assessment of suspected carcinogens in drinking water, Interim Report to Congress. Office of Toxic Substances (1975) (17) Krill RM, Sonzogni WC; J Amer Water Works Assoc 78: 70-5 (1986) (18) Steichen J et al; Ground Water Monit Rev 8: 153-60 (1988) (19) Andelman JB; Sci Total Environ 47: 443-60 (1985) (20) Takeoka GR et al; J Agric Food Chem 36: 553-60 (1988) (21) Heikes DL, Hopper ML; J Assoc Off Anal Chem 69: 990-8 (1986) (22) Heikes DL; J Assoc Off Anal Chem 70: 215-26 (1987) (23) Daft JL; Sci Total Environ 100: 501-18 (1991) (24) Rembold H et al; J Agric Food Chem 37: 659-62 (1989)]

Environmental Transport and Persistence:

Bioaccumulation: An experimental bioconcentration factor of 2 for DCE (1) indicates a low potential for bioconcentration in fish or aquatic organisms.

[(1) Barrows ME et al; Dyn Exposure Hazard Asses Toxic Chem, Ann Arbor, MI, Ann Arbor Sci. p.379-92 (1980)]

Volatilization/ Adsorption: According to a simple fugacity model, the mass distribution of DCE among the environmental compartments at equilibrium is 1.45% to water, 98.55% to air, and none to soil (1). The half-life for volatilization from a model river and lake are 1.4 hours and 4 days, respectively (2). Soil adsorption coefficients ranging from 30 to 152 can be estimated from the water solubility and log octanol/water partition coefficient of DCE, respectively (2), indicating moderate to high mobility in soil (3). Volatilization of DCE from both dry and moist soil is expected to be rapid in light of its high vapor pressure, high Henry's Law constant, and limited potential for adsorption to soil.

[(1) EPA; PCGEMS (Graphical Exposure Modeling System), PCENPART (Environmental Partitioning Model) (2) Lyman WJ et al; Handbook of Chemical Property Estimation Methods. Environmental Behavior of Organic Compounds. New York, NY: McGraw-Hill pp. 4.1-4.33 (1982) (3) Swann RL et al; Res Rev 85:17-28 (1983)]

Persistence: DCE reacts with photochemically-produced hydroxyl radicals in the atmosphere with an experimental rate constant of $2.20 \times 10^{-13} \text{ cm}^3/\text{molecule-sec}$ (1). Using an atmospheric hydroxyl radical concentration of $5 \times 10^5 \text{ molecule/cm}^3$, the estimated half-life for DCE in the atmosphere is approximately 50 days. DCE is expected to slowly biodegrade under both aerobic (2-5) and anaerobic (4, 6, 7) conditions in the environment, although high concentrations may be toxic to microorganisms (8, 9).

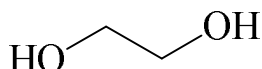
[(1) Atkinson R; Chem Rev 85: 69-201 (2) Oldenhuis R et al; Appl Environ Microbiol 55: 2819-36 (1989) (3) Lanzarone NA, McCarty PL; Ground Water 28: 910-19 (1990) (4) Watwood ME et al; Appl Environ Microbiol 57: 717-20 (1991) (5) Henson JM et al; FEMS Microbiol Ecol 59: 193-201 (1988) (6) Saint-Fort R; J Environ Sci Health A26: 13-62 (1991) (7) Jafvert CT, Wolfe NL; Environ Toxicol Chem 6: 827-37 (1987) (8) Blum DJW, Speece RE; Res J Water Pollut Contrl Fed 63: 198-207 (1991) (9) Colleran E et al; Water Sci Technol 25: 31-40 (1992)]

ETHYLENE GLYCOL

SUBSTANCE IDENTIFICATION

Synonyms: 1,2-Dihydroxyethane; 2-hydroxyethanol; 1,2-ethanediol

Structure:



CAS Registry Number: 107-21-1

Molecular Formula: C₂H₆O₂

CHEMICAL AND PHYSICAL PROPERTIES

Boiling Point: 197.6 °C

Melting Point: -13 °C

Molecular Weight: 62.07

Dissociation Constants: Not applicable

Log Octanol/Water Partition Coefficient (log K_{ow}): -1.36 (1)

Water Solubility: miscible (2)

Vapor Pressure: 0.0878 mm Hg @ 25 °C (2)

Henry's Law Constant: 6 x 10⁻⁸ atm-m³/mole (3)

Lower Explosive Limit: Not available

[(1) Hansch C, Leo AJ; Medchem Project Issue No 26 Claremont, CA: Pomona College (1985) (2) Riddick JA et al; Organic Solvents 4th ed. pp. 263-265. New York, NY: Wiley (1986) (3) Butler JAU, Ramchandani CN; J Chem Soc 95205 (1935)]

EXPOSURE PROFILE

Production: Ethylene glycol had a 1992 production volume of 2.2 billion pounds 7.4 billion pounds, of which 2.2 billion pounds were exported and an additional 400 million pounds were imported (1). Ethylene glycol is produced by Union Carbide (Taft, LA, Seadrift, TX, Prentiss, Canada, and Montreal, Canada), Dow (Plaquemine, LA, Fort Saskatchewan, Canada), PD Glycol (Beaumont, TX), Texaco (Port Neches, TX), Oxy Petrochemicals (Bayport, TX), Hoechst Cellanese (Clear Lake, TX), Shell (Gelsmar, LA), BASF (Gelsmar, LA) Quantum (Morris, IL), and Eastman (Longview, TX) (1). Of the production capacity listed above, 15.8% is Canadian.

[(1) Chemical Marketing Reporter; Chemical Profile: Ethylene Glycol. January 25, 1993]

Use: Ethylene glycol is used as an antifreeze in heating and cooling systems, a de-icing agent on bridges and airport runways, and a solvent in the paints and plastics industry (2, 3). It is used in hydraulic brake fluids, printer's inks, and inks for stamp pads and ball point pens (2, 3). Ethylene glycol is a reactant, along with dimethyl terephthalate, in the production of polyethylene terephthalate (PET) (4). Its pattern of use is: antifreeze (42%), polyester fiber (27%), PET bottles and other packaging material (12.5%), PET film (6%), and miscellaneous and other PET resin uses (12.5%) (1).

[(1) Chemical Marketing Reporter; Chemical Profile: Ethylene glycol. January 25, 1993 (2) Budavari D et al; The Merck Index 11th ed. p. 599. Rahway, NJ: Merck & Co Inc (1989) (3) Hawley CG; The Condensed Chemical Dictionary 10th ed. pp. 431-432. New York, NY: Van Nostrand Reinhold Co (1981) (4) Sattler, H; Ullmann's Encyclopedia of Industrial Chemistry A10:581]

Occupational Exposure: NIOSH (NOES Survey 1981-83) has statistically estimated that 1,133,792 workers are exposed to ethylene glycol in the United States (1). In a study of 543 workplaces in France between 1981 and 1985, ethylene glycol was found in 70 of 2,013 air samples, of which 43% exceed the VME (French exposure limit) (2). Ethylene glycol was found in conjunction with painting, printing, and serigraphy (2). The highest concentrations of ethylene glycol aerosol and vapor found in the breathing zone of workers spraying 50% ethylene glycol on bridges were 2.33 and 3.36 mg/m³, respectively (3). The workers spraying the bridges were in trucks. The maximum time weighted average (TWA) concentrations of ethylene glycol aerosol and vapor collected from bridges were 0.33 and 10.34 mg/m³, respectively (3). The mean TWA concentration of ethylene glycol in a nylon polyester filament and rayon staple facility was 2.59 ppm (6.67 mg/m³) (4).

[(1) NIOSH. National Institute for Occupational Safety and Health. National Occupational Exposure Survey (NOES). Computer printout March 29, 1989 (2) Ensminger A; Sampling of organic pollutants in the workplace atmosphere. Results. CAH Notes Doc 131: 299-301 (1988) (3) Abdelghani AA et al; Fate of ethylene glycol in the environment. FHWA/LA-90/228. Louisiana Department of Transportation and Development [NTIS PB90-264672] (1990) (4) Fajen JM; In-Depth Industrial Hygiene Report of the American Enka Company, Lowland, Tennessee, Report No. IWS-75-14SI. NIOSH, U.S. Department of Health and Human Services, Cincinnati, Ohio (1982)]

Consumer Exposure: Consumer exposure to ethylene glycol will result from its use in antifreeze and as a solvent in ballpoint pen inks and stamp pads. No data containing exposure levels or estimates of the number of exposed consumers or exposure concentrations were located.

Environmental Release and General Population Exposure: According to the 1991 Toxics Release Inventory (TRI), 17.5 million pounds of ethylene glycol were released to the environment, of which 60.8% was released into the atmosphere, 13.1% to water, and 5.2% to land (1). Ethylene glycol may enter the environment from its uses in de-icing runways and from spills and improper disposal of antifreeze, coolant, and solvents containing ethylene glycol (2).

[(1) U.S. EPA; Toxics Release Inventory (1992) (2) Lovell R; Organic chemical manufacturing Volume 9. EPA-450/3-80-028d (1980)]

Environmental Transport and Persistence:

Bioaccumulation: The bioconcentration factor (BCF) for ethylene glycol in fish (Golden ide) was reported to be 10 after 3 days of exposure (1). Ethylene glycol's low BCF indicates that it does not bioconcentrate in aquatic organisms. Crayfish exposed to ethylene glycol for 61 days bioconcentrated only minimal amounts of ethylene glycol and completely depurated it from their systems within 6 days (2).

[(1) Freitag D et al; Chemosphere 14: 1589-616 (1985) (2) Abdelghani AA et al; Fate of ethylene glycol in the environment. FHWA/LA-90/228. Louisiana Department of Transportation and Development [NTIS PB90-264672] (1990)]

Volatilization/ Adsorption: Because of its high solubility in water and low vapor pressure, ethylene glycol will partition into water. According to a simple fugacity model, the mass distribution of ethylene glycol among the environmental compartments is 0.0004 in air, 0.9995 in water, and 0.0001 in soil (2). Since ethylene glycol is miscible in water, it should have a very low adsorptivity to soil (1). The K_{oc} for ethylene glycol estimated from molecular structure is 0.04 (4). Absorption to five soils was negligible (3). Similarly, ethylene glycol's very low Henry's Law constant indicates that its volatilization from water will be very low (1). Since ethylene glycol has a low vapor pressure, it will not evaporate rapidly from soil.

[(1) Lyman WJ et al; Handbook of Chemical Estimation Methods Washington, DC: American Chemical Society pp. 4-1 to 4-33, 15-15 to 15-29 (1990) (2) U.S. EPA; PCGEMS (Graphical Exposure Modeling System), PCENPART (Environmental Partitioning Model) (3) Abdelghani AA et al; Fate of ethylene glycol in the environment. FHWA/LA-90/228. Louisiana Department of Transportation and Development [NTIS PB90-264672] (1990) (4) Meylan WM et al; Environ Sci Technol 26: 1560-7 (1992)]

Persistence: Vapor-phase ethylene glycol reacts with photochemically-produced hydroxyl radicals with a rate constant of $7.7 \times 10^{12} \text{ cm}^3/\text{molecule-sec}$ (1). Assuming a hydroxyl radical concentration of $5 \times 10^5/\text{cm}^3$, the atmospheric half-life would be 50 hours. Glycols are resistant to hydrolysis (2). There is a large body of information confirming the biodegradability of ethylene glycol in aerobic systems using activated sludge, sewage, and soil inocula. Degradation is essentially complete in <1-4 days; although 100% theoretical biological oxygen demand may not be realized for several weeks (3-12, 15). In a river die-away test, degradation was completed in 3 days at 20°C and 5-14 days at 8°C (13). No ethylene glycol was found in water, soil, and sediment around bridges sprayed with 50% ethylene glycol (15). Data are limited for anaerobic systems, but the evidence indicates that ethylene glycol also readily biodegrades under anaerobic conditions (14).

[(1) Atkinson R; Chem Rev 85: 69-201 (1985) (2) Lyman WJ et al; Handbook of Property Estimation Methods. Environmental Behavior of Organic Compounds Washington, DC: American Chemical Society pp. 7-1 to 7-48 (1990) (3) Bridie AL et al; Water Res 13: 627-30 (1979) (4) Conway RA et al; Environ Sci Technol 17: 107-12 (1983) (5) Haines JR, Alexander M; Appl Microbiol 29: 621-5 (1975) (6) Helfgott TB et al; An index of refractory organics. EPA 600/2-77-174 (1977) (7) Matsui S et al; Prog Water Technol 7: 645-59 (1975) (8) Means JL, Anderson SJ; Water Air Soil Pollut 16: 301-15 (1981) (9) Pitter P; Water Res 10: 231-5 (1976) (10)

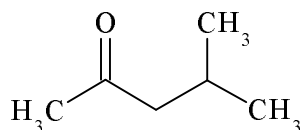
Price KS et al; J Water Pollut Control Fed 46: 63-77 (1974) (11) Schefer W, Waelchli O; Z Wasser Abwasser Forsch 13: 205-9 (1980) (12) Zahn R, Wellens H; Z Wasser Abwasser Forsch 13: 1-7 (1980) (13) Evans WH, David EJ; Water Res 8: 97-100 (1974) (14) Dwyer DF, Tiedje JM; Appl Environ Microbiol 46: 185-90 (1983) (15) Abdelghani AA et al; Fate of ethylene glycol in the environment. FHWA/LA-90/228. Louisiana Department of Transportation and Development [NTIS PB90-264672] (1990)]

METHYL ISOBUTYL KETONE

SUBSTANCE IDENTIFICATION

Synonyms: 4-Methyl-2-pentanone; MIBK; hexone

Structure:



CAS Registry Number: 108-10-1

Molecular Formula: C₆H₁₂O

CHEMICAL AND PHYSICAL PROPERTIES

Boiling Point: 116.8 °C

Melting Point: -84.7 °C

Molecular Weight: 100.18

Dissociation Constants: Not applicable

Log Octanol/Water Partition Coefficient (log K_{ow}): 1.16 (1)

Water Solubility: 20,400 mg/L @ 20 °C (2)

Vapor Pressure: 14.5 mm Hg @ 20 °C (3)

Henry's Law Constant: 9.4 x 10⁻⁵ atm-m³/mole (calculated from vapor pressure and water solubility)

Lower Explosive Limit: 1.4% @ 20 °C (4)

[(1) Meylan WM, Howard PH; Group contribution method for estimating octanol-water partition coefficients. SETAC Meeting Cincinnati, OH. Nov 8-12, (1992) (2) Ginnings PM et al; J Am Chem Soc 62: 1923-4 (1940) (3) Boublik T et al; The Vapor Pressures of Pure Substances. p. 481. Amsterdam: Elsevier (1984) (4) NIOSH; NIOSH Pocket Guide Chem Haz, 2nd prt p. 134 (1987)]

EXPOSURE PROFILE

Production: Methyl isobutyl ketone (MIBK) had a 1992 production volume of 175 million pounds; an additional 21.6 million pounds were imported (1). Exports were 35 to 42 million pounds a year (1). MIBK is produced by Shell (Deer Park, TX), Union Carbide (Institute, WV), and Eastman (Kingsport, TN) (1).

[(1) Chemical Marketing Reporter; Chemical Profile: Methyl isobutyl ketone. August 2, 1993]

Use: MIBK is an important solvent for vinyl, epoxy, and acrylic resins, for natural resins, and for nitrocellulose and dyes (2). It is also used as an extractant (2). Its use pattern is: surface coatings (66%), process solvent for pharmaceuticals, adhesives, and pesticides (15%), chemical production including rubber processing chemicals (15%), and miscellaneous (4%) (1).

[(1) Chemical Marketing Reporter; Chemical Profile: Methyl isobutyl ketone. August 2, 1993 (2) Siegel H, Eggerdorfer M; Ullmann's Encyclopedia of Industrial Chemistry A15: 77-95 (1990)]

Occupational Exposure: NIOSH (NOES Survey 1981-83) has statistically estimated that 467,763 workers are exposed to MIBK in the United States (1). Workers were exposed to mean time weighted average (TWA) exposures of 0.6 ppm (standard deviation 1.9 ppm) of MIBK during spray painting in spray booths (2). Highest sample and TWA values were 45 ppm and 8.8 ppm, respectively (2). Other occupational exposures include: 24 to 143 ppm for a screen washing booth in a custom silkscreen printed vinyl wall covering plant (3); and a mean of 1.7 ppm for car painters (4).

[(1) NIOSH. National Institute for Occupational Safety and Health. National Occupational Exposure Survey (NOES). Computer printout March 29, 1989 (2) Whitehead LW et al; Am Ind Hyg Assoc J 45: 767-72 (1984) (3) Almaguer D; Health Hazard Evaluation Report No. HETA-84-299-1543, Impressions Handprinters, Chicago, Illinois NIOSH, U.S. Department of Health and Human Services, Cincinnati, Ohio (1984) (4) Kurppa K, Husman K; Scand J of Work, Environ Health 8: 137-140 (1982)]

Consumer Exposure: MIBK was found in 64 of 1,039 household products surveyed from 65 product categories representing 8 product classes in a study of indoor air pollution chemicals (1, 3). Product classes likely to contain MIBK (% of products containing MIBK) are paint-related products (10.9%), adhesive-related products (4.3%), automotive products (3.8%), fabric and leather treatments (4.5%), oils, greases, and lubricants (3.9%), and cleaners for electronic equipment (3.6%) (3). The mean concentrations of MIBK in product classes *for products containing MIBK* are paint-related products (6.9%), adhesive-related products (5.0%), automotive products (2.9%), fabric and leather treatment (2.7%), and cleaners for electronic equipment (1.2%) (3). Product categories where products are likely to contain MIBK are spray paint, paint removers, paint thinners, carburetor and choke cleaners, adhesives, wood stains, varnishes, and finishes, primers, spot removers, spray shoe polish, fabric finishers, tape recorder cleaners, tire cleaner and paint, and silicone lubricants (1). This high occurrence of MIBK in household products indicates that there is a high potential for consumer exposure to MIBK. For 17 consumer products containing MIBK, consumer usage per product has been estimated to range from 7.2 to 112 million people (2).

[(1) Sack TM, Steele DH; Indoor air pollutants from household product sources. EPA: Environmental Monitoring Systems Laboratory. EPA/600/S4-91/025 (1991) (2) U.S. EPA; Multi-substance rule for the testing of neurotoxicity (proposed rule). 56 FR 9105 (March 4, 1991) (3) Sack TM et al; Atmos Environ 26: 1063-1070 (1992)]

Environmental Release and General Population Exposure: According to the 1991 Toxics Release Inventory (TRI), 27.7 million pounds of MIBK were released to the environment, of

which 98.2% was released into the atmosphere, 0.6% to land, and 0.6% to water (1). MIBK is found in exhaust gas from motor vehicles which indicates that there may be widespread exposure to the general population from traffic (2). MIBK occurs naturally in oranges, grapes, and vinegar (3), and is a volatile component of baked potatoes which indicates that there may be exposure from plant volatiles and food (4). MIBK has been detected in air in industrial areas at a median concentration of 270 ppt (5) and at a water treatment plant at <0.5-13 ppm (6). It has been detected, but not quantified, in river water (7, 8, 9). MIBK was reported in leachate from municipal landfills at 25-263 ppb (10, 11). MIBK has been identified in the effluent from at least one plant in each of the following industries: printing and publishing, coal mining, electronic, and organic chemicals (12).

[(1) U.S. EPA; Toxics Release Inventory (1992) (2) Hampton CV et al; Environ Sci Tech 16: 287-98 (1982) (3) Fenaroli Handbook of Flavor Ingredients 2nd ed, Volume 2 (1975) (4) Coleman EC et al; J Agric Food Chem 29: 42-8 (1981) (5) Brodzinsky R, Singh HB; Volatile Organic Chemicals in the Atmosphere: An Assessment of Available Data Menlo Park, CA: SRI International p. 23, 187 (1982) (6) Dunovant VS et al; J Water Pollut Control Fed 58: 886-95 (1986) (7) Great Lakes Water Quality Board; An Inventory of Chemical Substances Identified in the Great Lakes Ecosystem Volume 1 - Summary; Windsor Ontario, Canada (1983) (8) Ewing BB et al; Monitoring to detect previously unrecognized pollutants in surface waters. Appendix: Organic analysis data EPA 560/6-77-015 (1977) (9) Sheldon LS, Hites RA; Environ Sci Tech 12: 1188-94 (1978) (10) Sawhney BL, Kozlosku RP; J Environ Qual 13: 349-52 (1984) (11) Sawhney BL, Raabe JA; The Connecticut Agric Experiment Bull 833: 1-9 (1986) (12) Bursey JT, Pellizzari ED; Analysis of industrial wastewater of organic pollutants in consent survey EPA Contract No. 68-03-2867 (1982)]

Environmental Transport and Persistence:

Bioaccumulation: Bioconcentration factors (BCF) of 2-5 were estimated for MIBK using linear regression equations with the log K_{ow} and water solubility (1). These BCF values suggest that MIBK will not bioaccumulate significantly in aquatic organisms.

[(1) Lyman WJ et al; Handbook of Chemical Property Estimation Methods. New York, NY: McGraw Hill pp. 5-5 to 5-6 (1982)]

Volatilization/ Adsorption: According to a simple fugacity model, the mass distributions of MIBK among the environmental compartments are 0.85 in air, 0.15 in water, and 0.0001 in soil (4). The volatilization half-life for MIBK from a model river 1 m deep with a current of 1 m/s and a wind of 3 m/s is estimated to be 12.3 hours (1). Similarly, the volatilization half-life for a model lake 1 m deep with a 0.05 m/s current and 0.5 m/s wind is 6.8 days. The overall mass-transfer coefficient for the volatilization of methyl isobutyl ketone from water in a stirred (557-2020 rpm) laboratory bath at 25 °C was found to range from 0.497 to 1.11 m/day (2). Based on these values, the volatilization half-life of MIBK from water 1 m deep has been estimated to be 15-33 hours. Soil adsorption coefficients (K_{oc}) of 19-106 are estimated for MIBK using linear regression equations based on the log K_{ow} and water solubility (1). These K_{oc} values suggest that MIBK would be highly mobile in soil and would not adsorb significantly to suspended solids and sediments in water bodies (3). The low Henry's Law constant and low adsorption to soil indicates that MIBK may readily volatilize from soil.

[(1) Lyman WJ et al; Handbook of Chemical Property Estimation Methods New York, NY: McGraw-Hill p. 4-9 to 4-10, 15-1 to 15-32 (1982) (2) Rathbun RE, Tai DY; Water Air Soil Poll 17: 281-93 (1982) (3) Swann RL et al; Res Rev 85: 17-28 (1983) (4) U.S. EPA; PCGEMS (Graphical Exposure Modeling System), PCENPART (Environmental Partitioning Model)]

Persistence: MIBK reacts with photochemically-produced hydroxyl radicals in the atmosphere at a rate of $14.1 \times 10^{-12} \text{ cm}^3/\text{molecule-s}$ (1). Assuming a hydroxyl radical concentration of $5 \times 10^5 \text{ radicals/cm}^3$, the half-life of MIBK in the atmosphere will be 27 hours. MIBK in cyclohexane exhibits strong absorption of UV light $>290 \text{ nm}$ (3), suggesting that MIBK has the potential to undergo direct photolysis in the environment. Assuming that the photolysis rate is similar to that of methyl ethyl ketone, the photolysis rate and half-life (solar zenith angle of 30°) will be $12.5 \times 10^6 \text{ s}^{-1}$ and 15 hours, respectively (2). Ketones are resistant to chemical hydrolysis (4). MIBK is biodegradable in screening studies (4-9). MIBK incubated with settled domestic sewage as seed was found to have 5-, 10-, and 40-day BOD values of 4.4%, 49.3%, and 64.8%, respectively (7). Other studies indicate that freshwater seeded with settled domestic sewage exerted 5- and 20-day BODs of 4.4-76% and 69%, respectively (4, 5, 6). In seeded synthetic sea water, 5- and 20-day BODs of 15-31% and 53%, respectively, have been observed (5, 6). MIBK undergoes anaerobic biodegradation in an aquifer slurry after 3-4 weeks acclimation (10); 46% of the theoretically expected amount of methane was recovered.

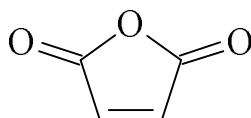
[(1) Atkinson R; Chem Rev 85: 69-201 (1985) (2) Cox RA et al; Environ Sci Technol 15: 587-92 (1981) (3) Sadtler; Standard UV Spectra No. 21; Philadelphia: Sadtler Res Lab (1961) (4) Bridie AL et al; Water Res 13: 627-30 (1974) (5) Takemoto S et al; Suishitsu Odaku Kenkyu 4: 80-90 (1981) (6) Price KS et al; J Water Pollut Control Fed 46: 63-77 (1974) (7) Ettinger MB; Ind Eng Chem 48: 256-9 (1956) (8) Ludzack FJ, Ettinger MB; J Water Poll Control Fed 32: 1173-200 (1960) (9) Sasaki S; pp. 283-98 in Aquatic Pollutants: Transformation and Biological Effects; Hutzinger O; Pergamon Press (1978) (10) Suflita JM, Mormile MR; Environ Sci Technol 27: 976-978 (1993)]

MALEIC ANHYDRIDE

SUBSTANCE IDENTIFICATION

Synonyms: 2,5-Furandione; *cis*-butenedioic anhydride

Structure:



CAS Registry Number: 108-31-6

Molecular Formula: C₄H₂O₃

CHEMICAL AND PHYSICAL PROPERTIES

Boiling Point: 202.0 °C

Melting Point: 52.8 °C

Molecular Weight: 98.06

Dissociation Constants: Not applicable

Log Octanol/Water Partition Coefficient: Hydrolyzes (3)

Water Solubility: Hydrolyzes (1)

Vapor Pressure: 0.41 mm Hg @ 25 °C (2)

Henry's Law Constant: Not applicable

Lower Explosive Limit: 1.4% @ 25 °C (4)

[(1) Weast RC; Handbook of Chemistry and Physics 67th ed. (1986) (2) Cupitt LT; Fate of toxic and hazardous materials in the air environment; EPA 600/3-80-084 (1980) (3) Meylan WM, Howard PH; Group contribution method for estimating octanol-water partition coefficients. SETAC Meeting Cincinnati, OH. Nov 8-12, (1992) (4) Sax NI; Dangerous Properties of Industrial Materials 6th Edition, p. 1726 (1984)]

EXPOSURE PROFILE

Production: There were 382 million pounds of maleic anhydride produced in 1991 of which 20.9 million pounds were exported; an additional 2.8 million pounds were imported (1). Maleic anhydride is produced by Monsanto (Pensacola, FL), Amoco (Joliet, IL), Miles (Houston, TX), Ashland (Neal, WV), and Aristech (Neville Island, PA) (1). Maleic anhydride is available as briquettes and capulets, and in molten form (2).

[(1) Chemical Marketing Reporter; Chemical Profile: Maleic Anhydride. July 6, 1992 (2) Chemcyclopedia93; p. 90 Washington, DC: American Chemical Society (1992)]

Use: Maleic anhydride is used primarily in the production of unsaturated polyester resins (60%) (1). It is also used to make lubricating oil additives (10%), copolymers (7%), fumaric acid (6%), agricultural chemicals (5%), and maleic acid (2%) (1). Other uses, including sulfosuccinic acid esters and alkenyl succinic anhydrides production, consume 10% of production (1). Up to 10 mole percent of maleic anhydride may be substituted for phthalic anhydride in alkyd resins (2). Polyester and alkyd resins, in particular, are used to make fiberglass reinforced plastics in the construction and electrical industries, in pipeline and marine construction (3), and in textile finishing (4). Agricultural chemicals that are produced from maleic anhydride include the pesticides captan and malathion, and the growth inhibitor maleic acid hydrazide (3). Maleic anhydride is also added to drying oils to reduce the drying time and improve the coating qualities of lacquers (3).

[(1) Chemical Marketing Reporter; Chemical Profile: Maleic Anhydride. July 6, 1992 (2) Lin KF; Kirk-Othmer Encyclopedia of Chemical Technology, 4th ed. 2: 58 (1992) (3) Lohbeck K et al; Ullmann's Encyclopedia of Industrial Chemistry A16: 54-59 (1990) (4) Chemcyclopedia93; p. 90 Washington, DC: American Chemical Society (1992)]

Occupational Exposure: NIOSH (NOES Survey 1981-83) has statistically estimated that 37,897 workers are exposed to maleic anhydride in the United States (1). Workers are most likely to be exposed to maleic anhydride via inhalation of dust or vapor or dermal contact in production facilities or factories that produce unsaturated polyester resins, lubricating oils, and other chemicals that use maleic anhydride. Of special concern is loading and unloading maleic anhydride solids and exposure to vapor from molten material. One worker was acutely affected from exposure to maleic anhydride minutes after loading alkyd resins in a reactor; no environmental levels were reported (4). One Russian study has shown that maleic anhydride may be emitted from fiberglass composites during heating at 100°C to 160 °C (5). There may be some occupational exposure to maleic anhydride under conditions where fiberglass composites are heated.

The waste water stream from the "bottoms" of the purification system for the most common maleic anhydride production method, C₄-oxidation (2), contains maleic anhydride (3). However, it is not clear whether there is a potential occupational exposure from this source. While maleic anhydride hydrolyzes rapidly in water, hydrolysis may be much less rapid in industrial waste streams which have a large non-aqueous component.

[(1) NIOSH. National Institute for Occupational Safety and Health. National Occupational Exposure Survey (NOES). Computer printout March 29, 1989 (2) Lohbeck K et al; Ullmann's Encyclopedia of Industrial Chemistry A16: 54-59 (1990) (3) Liepins R et al; Industrial process profiles for environmental use. Chapter 6. The industrial organic chemical industry pp. 6-176 to 6-177. EPA-600/2-77-032f (1977) (4) Lee HS et al; British J Indust Med 48: 283-285 (1991) (5) Stankevich KI, Ovdienko TL; Plasticheskie Massy No. 7 (1977)]

Consumer Exposure: No information was found which would indicate that maleic anhydride is used in consumer products.

Environmental Release and General Population Exposure: According to the 1991 Toxics Release Inventory (TRI), 460,859 pounds of maleic anhydride were released to the environment, of which 99.6% was released into the atmosphere (1).

[(1) U.S. EPA; Toxics Release Inventory (1992)]

Environmental Transport and Persistence:

Bioaccumulation: Maleic anhydride hydrolyzes much too rapidly (see Persistence, below) for bioconcentration in aquatic organisms to be a concern.

Volatilization/ Adsorption: Maleic anhydride hydrolyzes rapidly in water (see Persistence, below) and most likely hydrolyzes rapidly in soil; and thus, volatilization from water and soil, and leaching in soil would not be important. Due to its rapid hydrolysis in water and likely rapid hydrolysis in soil, the atmosphere appears to be the environmental compartment where maleic anhydride will persist the longest.

Persistence: Maleic anhydride hydrolyzes rapidly in water at room temperature to produce maleic acid. The first order rate constants in initial neutral solutions are $1.83 \times 10^{-2} \text{ s}^{-1}$ and $3.14 \times 10^{-2} \text{ s}^{-1}$ at 18.6 °C and 25.1 °C, respectively (1). The respective half-lives are 22 and 38 seconds, respectively.

When maleic anhydride was exposed to an atmosphere with 96% relative humidity at 22 °C, it was completely hydrolyzed to maleic acid in 21 hours; however, no hydrolysis occurred in 46 hours at 50% relative humidity (6). Hydrolysis involves ions and therefore, should not occur in the vapor phase. Maleic anhydride was probably absorbed into water droplets in the atmosphere or on the walls of the appropriate chamber where the hydrolysis occurred.

Maleic anhydride has been characterized as biodegradable during biological sewage treatment (8). In one report, 99% removal was achieved in 4 hours by activated sludge (9). Others report 40-60% theoretical BOD in 5 days with sewage inoculum (10, 11). The initial step in the biodegradation would be the chemical hydrolysis of maleic anhydride to maleic acid.

The gas/particle partitioning of semivolatile organic compounds in atmosphere depends on the vapor pressure of the organic compound and the concentration of total suspended particulate matter (2). According to this theory, atmospheric maleic anhydride will primarily be found in the vapor phase. Maleic anhydride reacts with both hydroxyl radicals and ozone in the atmosphere. Estimated hydroxyl rate constants estimated from molecular structure are $2.24 \times 10^{-12} \text{ cm}^3/\text{molecule-s}$ (3) and $46 \times 10^{-12} \text{ cm}^3/\text{molecule-s}$ (4). Assuming a hydroxyl radical concentration of $5 \times 10^5 \text{ radicals/cm}^3$, the respective half-lives will be 7.2 days and 8.4 hours. The rate constants for reaction with ozone are estimated to be $0.175 \times 10^{-17} \text{ cm}^3/\text{molecule-s}$ (3) and $4.9 \times 10^{-17} \text{ cm}^3/\text{molecule-s}$ (5). Assuming an

ozone concentration of 7×10^{11} molecules/cm³, the respective half-lives will be 6.5 days and 5.6 hours. At night, maleic anhydride may react with NO₃ radicals with an estimated rate constant of 1.02×10^{-13} cm³/molecule-s (4). Assuming an NO₃ radical concentration of 2.4×10^8 molecules/cm³, the half-life of maleic anhydride will be 7.9 hours. Although maleic anhydride absorbs UV radiation above 290 nm (7), no information was found concerning direct photolysis.

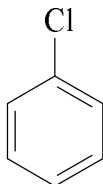
[(1) Bunton CA et al; J Chem Soc 1963: 2918-26 (1963) (2) Bidleman T; Environ Sci Technol 22: 361-367 (1988) (3) Meylan WM, Howard PH; Chemosphere 26: 2293-9 (1993) (4) Grosjean D, Williams EL II; Atmos Environ 26A: 1395-1405 (1992) (5) Grosjean D; J Air Waste Manage Assoc 40: 1664-1668 (1990) (6) Rosenfeld JM, Murphy CB; Talenta 14: 91-96 (1967) (7) Sadtler Index 163 UV (8) Thom NS, Agg AR; Proc R Soc London B 189: 347-57 (1975) (9) Matsui S et al; Prog Water Technol 7: 645-59 (1975) (10) Heukelekian H, Rand MC; J Water Pollut Control Assoc 29: 1040-53 (1955) (11) Verschueren K; Handbook of Environmental Data on Organic Chemicals; 2nd ed New York, NY: Van Nostrand Reinhold p. 803 (1983)]

CHLOROBENZENE

SUBSTANCE IDENTIFICATION

Synonyms: MCB; monochlorobenzene, phenyl chloride

Structure:



CAS Registry Number: 108-90-7

Molecular Formula: C₆H₅Cl

CHEMICAL AND PHYSICAL PROPERTIES

Boiling Point: 132 °C

Melting Point: -45.6 °C

Molecular Weight: 112.56

Dissociation Constants: Not applicable

Log Octanol/Water Partition Coefficient (log K_{ow}): 2.84 (1)

Water Solubility: 471.7 mg/L @ 25 °C (2)

Vapor Pressure: 11.9 mm Hg @ 25 °C (3)

Henry's Law Constant: 3.45 x 10⁻³ atm-m³/mole (4)

Lower Explosive Limit: 1.3% @ 150 °C (5)

[(1) Hansch C, Leo AJ; Medchem Project Issue No 26 Claremont, CA: Pomona College (1985) (2) Mackay D et al; Environ Sci Tech 13: 333-6 (1979) (3) Daubert TE, Danner RP; Data Compilation Tables of Properties of Pure Compounds Amer Institute of Chem Eng (1985) (4) Mackay D, Shiu WY; J Phys Chem Ref Data 19: 1175-99 (1981) (5) Sax NI; Dangerous Properties of Industrial Materials, 6th Edition p. 363 (1984)]

EXPOSURE PROFILE

Production: The U.S. production of monochlorobenzene (MCB) in 1991 was 210 million pounds (1). Chlorobenzene is produced by Monsanto Co. (Sauget, IL), Standard Chlorine of Delaware, Inc. (Delaware City, DE), and PPG Industries, Inc. (Natum, WV) (1, 2).

[(1) USITC; Synthetic Organic Chemicals. United States Production and Sales, 1991. USITC Publication 2607. pp. 3-2, 3-4. February 1993 (2) SRI International; 1993 Directory of Chemical Producers, United States of America p. 519 (1993)]

Use: MCB is used largely in the production of nitrochlorobenzene (41%), which is used in the manufacture of dyes and pigments, rubber processing chemicals, pesticides, and pharmaceuticals (1). MCB is also used as a solvent, especially in herbicide formulations and other agricultural products (1). Formerly, large amounts of chlorobenzene were used to manufacture phenol, aniline, and DDT. These uses, however, have essentially disappeared due to the adoption of new processes and the phase-out of DDT (1).

[(1) Bryant JG; Kirk-Othmer Encyclopedia of Chemical Technology, 4th ed. 6: 87-100 (1993)]

Occupational Exposure: NIOSH (NOES Survey 1981-83) has statistically estimated that 17,056 workers are exposed to chlorobenzene in the United States (1). Personal air samples at a large MCB production plant (Dow, Midland, MI) ranged from 0.25 to 1.90 ppm in samples that had detectable MCB levels (2). Long term air samples contained 0.21 to 10.5 ppm of MCB (2). Chlorobenzene concentrations at the Du Pont Chamber Works in Deepwater, NJ ranged from non-detectable to 1.9 mg/m³ (0.40 ppm) (3).

[(1) NIOSH. National Institute for Occupational Safety and Health. National Occupational Exposure Survey (NOES). Computer printout March 29, 1989 (2) Crandall MS; In-depth survey of MCB and methyl chloride exposure at the Dow Chemical Company, Midland, Michigan NIOSH/00094286 (1980) (3) Fannick N; Toxic evaluation of inhaled chlorobenzene (monochlorobenzene). NIOSH HE-77-099-726 (1977)]

Consumer Exposure: In a study of indoor air pollution chemicals, chlorobenzene was not found in any of the 1043 household products surveyed from 81 product categories at concentrations greater than or equal to 0.1% by weight (1). This suggests that people are not exposed to chlorobenzene in consumer products.

[(1) Sack TM, Steele DH; Indoor air pollutants from household product sources. EPA: Environmental Monitoring Systems Laboratory. EPA/600/S4-91/025 (1992)]

Environmental Release and General Population Exposure: According to the 1991 Toxics Release Inventory (TRI), 2.58 million pounds of chlorobenzene were released to the environment, of which 92.9% was released into the atmosphere (1). Almost all of the remaining chlorobenzene was injected underground (1). Chlorobenzene concentrations in air in U.S. cities typically range from 0.0 to 0.8 ppb, although a maximum value of 12 ppb has been observed (3-6). In the New Jersey Airborne Toxic Elements and Organic Substances (ATEOS) program in which three cities were studied in summer and winter, chlorobenzene was detected in 91-100% of samples (detection limit 0.005 ppb) (14). Mean levels ranged from 0.07 to 0.22 ppb. In an EPA study of volatile air pollutants in six public buildings, chlorobenzene was "rarely detected" both inside and outside the buildings (12). Chlorobenzene was found in 9 of 10 finished drinking water supplies surveyed by the U.S. EPA; drinking water in Terrebonne Parish, LA and New York City contained 5.6 and 4.7 ppb, respectively (7). Chlorobenzene was occasionally found in drinking water in Los Angeles, CA (5-13% of samples) and Contra Costa, CA (6% of samples) (15). Chlorobenzene may be formed during chlorination of drinking water (7). Chlorobenzene was detected in 9.6% of surface water samples in the Ohio River Basin (1980-1981), but only 0.01%

of the samples were >1 ppb; the maximum concentration was >10 ppb (8). In 14 Industrial River Basins (1975-76), 5% of surface water samples contained 1-4 ppb of chlorobenzene (9). The concentration in the Calcasieu River, LA, near the outfall of a chemical plant was 18 ppt (13). In a 1981-82 survey of 945 wells scattered throughout the U.S., only 1 contained chlorobenzene; the concentration in the positive well was 2.7 ppb (10). Chlorobenzene was not found in any of the 1,791 community and private wells surveyed in Wisconsin (11). The concentration of chlorobenzene in 42 samples of mother's milk from women living near manufacturing plants or industrial facilities ranged from trace amounts to 10 ppb, with a mean of 0.37 ppb (2).

[(1) U.S. EPA; Toxics Release Inventory (1992) (2) Erickson MD et al; Acquisition and chemical analysis of mothers milk for selected toxic substances pp. 164 EPA 560/13-80-029 (1980) (3) Bozzelli JW et al; Analysis of selected toxic and carcinogenic substances in ambient air in New Jersey. State of NJ, Dept Environ Protect pp. 1-24 (1980) (4) Singh HB et al; Atmos Environ 15: 601-12 (1981) (5) Singh HB et al; Atmospheric measurements of selected hazardous organic chemicals EPA-600/3-81-032 (1981) (6) Pellizzari ED; Formulation of preliminary assessment of halogenated organic compounds in man and environmental media EPA 560/13-79-006 (1979) (7) National Academy of Sciences; Drinking Water and Health 4: 709 (1977) (8) Ohio River Valley Water Sanit Comm; Assessment of Water Quality Conditions. Ohio River mainstream 1980-81. Cincinnati, OH (1982) (9) Ewing BB et al; Monitoring to Detect Previously Unrecognized Pollutants in Surface Waters EPA-560/6-77-015a pp. 1-5, 72-74 (1979) (10) Westrick JJ et al; J Amer Water Works Assoc 76: 52-9 (1984) (11) Krill RM, Sonzogni WC; J Amer Water Works Assoc 78: 70-5 (1986) (12) Sheldon L et al; Indoor air quality in public buildings. Volume II. EPA/600/6-88/009b. Research Triangle Park, NC: EPA, Environmental Monitoring Systems Lab. pp. 1-3, 132-133 (1988) (13) Pereira WE et al; Environ Sci Technol 22: 772-778 (1988) (14) Harkov R et al; Sci Tot Environ 38: 259-274 (1984) (15) Wallace LA et al; Atmos Environ 22: 2141-2163 (1988)]

Environmental Transport and Persistence:

Bioaccumulation: The log BCF for chlorobenzene in several species of fish ranged from 1 to 2.65 (1-4). Therefore, MCB has a low to moderate potential for bioconcentrating in fish.

[(1) Kenaga EE; Bull Environ Safety 4: 26-38 (1980) (2) Veith GD et al; J Fish Board Canada 36: 1040-48 (1979) (3) Kawasaki M; Ecotoxicol Environ Safety 4: 444-54 (1980) (4) Kitano M; OECD Tokyo Mtg Ref Book TSU-No 3 (1978)]

Volatilization/ Adsorption: According to a simple fugacity model, chlorobenzene will distribute almost entirely to air (99.98%) (3). The volatilization half-life for chlorobenzene from a model river 1 m deep with a current of 1 m/s and a wind of 3 m/s is estimated to be 3.37 hours (1). Similarly, the volatilization half-life for a model lake 1 m deep with a 0.05 m/s current and 0.5 m/s wind is 4.3 days. Soil adsorption coefficients, K_{oc} , for chlorobenzene range from 147 to 389 (5,6). A K_{oc} of 268 is predicted on the basis of molecular structure (4). These K_{oc} values suggest that chlorobenzene is in a medium mobility class and would adsorb moderately to soil and sediment (2).

[(1) Lyman WJ et al; Handbook of Chemical Property Estimation Methods Washington, DC: American Chemical Society p. 4-9 to 4-10, 15-1 to 15-32 (1990) (2) Swann RL et al; Res Rev 85: 17-28 (1983) (3) U.S. EPA; PCGEMS (Graphical Exposure Modeling System), PCENPART (Environmental Partitioning Model) (4) Meylan WM et al; Environ Sci Technol 26: 1560-7 (1992)]

Persistence: Chlorobenzene absorbs light in the 290-310 nm region of the spectrum (2) and will photolyze in the troposphere (2) as well as in the surface water (3). However, the rate of photolysis is predicted to be low due to the poor overlap of the solar spectrum with the absorption spectrum (5). Chlorobenzene reacts with photochemically-produced hydroxyl radicals in the atmosphere with a rate of $7.7 \times 10^{13} \text{ cm}^3/\text{molecule-s}$ (1). Assuming a hydroxyl radical concentration of $5 \times 10^5 \text{ radicals/cm}^3$, the half-life of chlorobenzene in the atmosphere will be 21 days. The rate of reaction is expected to be higher in the presence of nitrogen oxides (smog situations) (4). Chlorobenzene is biodegraded by many bacteria and fungi in the environment (7-10). While biodegradation in soil and water is often slow, temperature and acclimation of microorganisms can increase the biodegradation rate (7-11). The biodegradation half-life has been reported to be 150 days in river water and 75 days in sediment (12). No significant mineralization occurred in soil in 8 months (13). The percent biodegradation of chlorobenzene in a municipal wastewater treatment plant with a 5.1 hour hydraulic retention time was 95.1% (14).

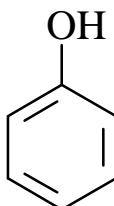
[(1) Atkinson R; J Phys Chem Ref Data. Monograph 1 (1989) (2) Uyetta M et al; Nature 264: 583-4 (1976) (3) Tissot A et al; Chemosphere 12: 859-72 (1983) (4) Kanno S, Nojima K; Chemosphere 8: 225-32 (1979) (5) Bunce NJ et al; Environ Sci Technol 23: 213-218 (1989) (6) Walton BT et al; J Environ Qual 21: 552-558 (1992) (7) Schwarzenbach RP, Westfall J; Environ Sci Technol 15: 1360-1367 (1981) (8) Haider K et al; Arch Microbiol 96: 183-200 (1974) (9) Ballschmitter K, Scholz C; Chemosphere 9: 457-67 (1980) (10) Smith RV, Rosazza JP; Arch Biochem Biophys 161: 551-8 (1974) (11) Tabak HH et al; J Water Pollut Control Fed 53: 1503-18 (1981) (12) Wakeham SG et al. Environ Sci Technol 17: 611-617 (1983) (13) Lee RF, Ryan CC; Microbial degradation of pollutants in the marine environments pp. 443-450. EPA/600/9-79-012 (1979) (14) Aelion CM et al; Appl Environ Microbiol 53: 2212-2217 (1987) (15) Namkung E, Rittman BE; J WPCF 59: 670-678 (1987)]

PHENOL

SUBSTANCE IDENTIFICATION

Synonyms: Hydroxybenzene; carbolic acid; phenyl alcohol

Structure:



CAS Registry Number: 108-95-2

Molecular Formula: C₆H₆O

CHEMICAL AND PHYSICAL PROPERTIES

Boiling Point: 182 °C

Melting Point: 40.9 °C

Molecular Weight: 94.11

Dissociation Constants: 1.28x10⁻¹⁰ at 20 °C (pK_a= 10.31) (1)

Log Octanol/Water Partition Coefficient (log K_{ow}): 1.46 (2)

Water Solubility: 82,800 mg/L at 25 °C (3)

Vapor Pressure: 0.35 mm Hg at 25 °C (4)

Henry's Law Constant: 3.33x10⁻⁷ at 25 °C (5)

Lower Explosive Limit: Not available

[(1) Chuchani G, Frohlich A; J Chem Soc B: 1417-20 (1971) (2) Hansch C, Leo AJ; Medchem Project Issue No 26 Claremont, CA: Pomona College (1985) (3) Southworth GR, Keller JL; Water Air Soil Poll 28: 239-48 (1986) (4) Jones AH; J Chem Eng Data 5: 196-200 (1960) (5) Gaffney JS et al; Environ Sci Technol 21: 519-24 (1987)]

EXPOSURE PROFILE

Production: In 1993, the U.S. demand for phenol stood at 3.9 billion pounds (excluding imports), of which 230-350 million pounds were exported (1). The current U.S. capacity stands at 4.17 billion pounds (1, 2). Phenol producers include Allied Signal (Frankford, PA), Aristech (Haverhill, OH), BTL (Blue Island, IL), Dakota Gasification (Beulah, ND), Dow (Freeport, TX), General Electric (Mount Vernon, IN), Georgia Gulf (Pasadena, TX, and Plaquemine, LA), Kalama (Kalama, WA), Merichem (Houston, TX), Shell (Deer Park, TX), and Texaco (El Dorado, KS) (1, 2).

[(1) Chemical Marketing Reporter; Chemical Profile: Phenol. p. 49, September 13, 1993 (2) SRI International; 1993 Directory of Chemical Producers, United States of America pp. 819-20 (1993)]

Use: Phenol's largest use is as a synthetic intermediate; it is a feedstock for the manufacture of Bisphenol A (35%), phenolic resins (34%), caprolactam (15%), aniline (5%), alkylphenols (5%), and xylenols (5%) (1). One percent of phenol production is distributed over a variety of uses (1) which include as a general disinfectant, an additive in germicidal paints and slimicides, a selective solvent for refining lubricating oils (2, 3), and in numerous medicinal and over-the-counter health and beauty aids (4, 5, 6, 7).

[(1) Chemical Marketing Reporter; Chemical Profile: Phenol. p. 49, September 13, 1993 (2) Budavari D et al; The Merck Index 11th ed. p. 1150 Rahway, NJ: Merck & Co. Inc (1989) (3) Hawley CG; The Condensed Chemical Dictionary 10th ed. p. 796 New York, NY: Van Nostrand Reinhold Co (1981) (4) Physicians Desk Reference 45th ed. pp. 1700, 1701, 1789, 1790, 2312 Oradel, NJ: Medical Economics Data (1991) (5) Douglass CC; J Assoc Off Anal Chem 55: 610-12 (1972) (6) U.S. EPA; Ambient Water Quality Criteria Document for Phenol. EPA 44/5-80-066. OHEA, ECAO, Cincinnati, OH (1980) (7) Musto JD et al; J Pharm Sci 66: 1201-2 (1977)]

Occupational Exposure: NIOSH (NOES Survey 1981-1983) has statistically estimated that 192,739 workers are exposed to phenol in the United States (1). General air samples at a brake assembly plant had phenol concentrations of 0.025-0.042 ppm (2). Phenol has been detected as a volatile degradation product of plastic (PVC) welding operations (3). An airplane interior part manufacturing plant, which used fiberglass wrap, had maximum phenol concentrations of 0.39 ppm (1.5 mg/m³) (4). General ambient air concentrations at a steel mill ranged from 0.01 to 0.05 ppm (0.04 to 0.20 mg/m³) (5). Phenol concentrations were below 0.01 ppm during oil sludge removal and maintenance activities at the Alyeska Pipeline Water Treatment Facility (6). Phenol concentrations up to 0.17 ppm (0.64 mg/m³) were measured during the production of refractory bricks (7). Occupational exposure to phenol by dermal contact has also been associated with phenol/formaldehyde resins (8, 9), and the manufacture of fiberglass (10). Phenol is formed by the thermal degradation of steel protective paints (11), and welding or flame cutting of painted metals may lead to inhalation exposure during these operations.

Room concentrations of phenol were measured at 1.3-5.0 ppm (12) and 0.002-3.2 ppm (0.01-12.2 mg/m³) (13) during cadaver dissection in gross anatomy courses at dental school. The analysis of personal samples showed that maximum personal concentrations of 0.55 ppm were found for embalmers (14). The use of hospital cleaning products may also lead to phenol exposure by either inhalation or dermal contact (15).

[(1) National Institute for Occupational Safety and Health (NIOSH) National Occupational Exposure Survey (NOES). Computer printout March 29, 1989 (2) Almaguer D; Health Hazard Evaluation Report No. HETA-85-048-049-1658, Lausen Engine Division, New Holstein, WI. Health Evaluation and Technical Assistance Branch, NIOSH, Cincinnati, OH (1985) (3) Andersson B; J Chromat 445: 353-61 (1988) (4) Gunter BJ et al; Health Hazard Evaluation Report No. HETA-88-294-1974, Boeing Aircraft, Seattle, WA. Hazard Evaluations and Technical Assistance Branch, NIOSH, U.S. Department of Health and Human Services, Cincinnati, OH (1989) (5) Gunter BJ; Health Hazard Evaluation Report No. HETA-86-034-1712, C F and I Steel, Pueblo, CO. Hazard Evaluations and Technical Assistance Branch, NIOSH, U.S. Department of Health and Human Services, Cincinnati, OH (1986) (6) Apol AG, Singal M; Health Hazard Evaluation Report No. HETA-86-132-1780, Alyeska Pipeline Service Company, Valdez, AK. Health Evaluation and Technical Assistance Branch, NIOSH, Cincinnati, OH (1987) (7) Murphy DC, Lucas C; Health Hazard Evaluation Report, No.

HETA-81-411-1182, Corhart Refractory, Louisville, KY. Hazard Evaluations and Technical Assistance Branch, NIOSH, Cincinnati, OH (1982) (8) Bruze M; Contact Dermatitis from Phenol-Formaldehyde Resins. Occupational and Industrial Dermatology, 2nd ed, H. I. Maibach, Ed; Chicago: Year Book Medical Publishers, Inc. pp. 430-435 (1987) (9) Fousseureau J et al.; Plastic Materials In: Occupational Contact Dermatitis, Clinical and Chemical Aspects, Philadelphia, PA, W. B. Saunders Company, pp. 216-37 (1982) (10) Cornwell RJ; Hazard Evaluation and Technical Assistance Report No. RDHETA-90-145-2086, MAP International, Fairmont, WV (1990) (11) Henriks-Eckerman M et al; Am Ind Hyg Assoc 51: 241-4 (1990) (12) Boiano JM; Health Hazard Evaluation Report No. HETA-84-098-1497, University of Pennsylvania Medical Education Building, Philadelphia, PA. Health Evaluation and Technical Assistance Branch, NIOSH, Cincinnati, OH (1984) (13) Gunter BJ, Thoburn TW; Health Hazard Evaluation Report, No. HETA-82-045-1108, University of Colorado Medical School, Denver, CO. Hazard Evaluations and Technical Assistance Branch, NIOSH, Cincinnati, OH (1982) (14) Stewart PA et al; Appl Occup Environ Hyg 7: 532-40 (1992) (15) Apol AG, Cone J; Health Hazard Evaluations Report, No. HETA-82-53-1263, Bay Area Hospital Coos Bay, OR. Health Evaluation and Technical Assistance Branch, NIOSH, Cincinnati, OH (1983)]

Consumer Exposure: Consumer exposure to phenol may occur during the use of commercial products that use it including general disinfectants, germicidal paints, and slimicides (1, 2). The presence of phenol in medicinal applications such as ointments, ear and nose drops, mouthwashes, gargles, toothache drops, analgesic rubs, throat lozenges and sprays, antifungal foot powders, and antiseptic lotions (3, 4, 5, 6) will lead to consumer exposure by those who use these products.

[(1) Budavari D et al; The Merck Index 11th ed. p. 1150 Rahway, NJ: Merck & Co. Inc (1989) (2) Hawley CG; The Condensed Chemical Dictionary 10th ed. p. 796 New York, NY: Van Nostrand Reinhold Co (1981) (3) Physicians Desk Reference 45th ed. pp. 1700, 1701, 1789, 1790, 2312 Oradel, NJ: Medical Economics Data (1991) (4) Douglass CC; J Assoc Off Anal Chem 55: 610-12 (1972) (5) U.S. EPA; Ambient Water Quality Criteria Document for Phenol. EPA 44/5-80-066. OHEA, ECAO, Cincinnati, OH (1980) (6) Musto JD et al; J Pharm Sci 66: 1201-2 (1977)]

Environmental Release and General Population Exposure: According to the 1991 Toxics Release Inventory (TRI), 10 million pounds of phenol were released to the environment, of which 63% was released into the atmosphere, 1.6% to water, 31.9% to underground injection, and 3.2% to land (1). Phenol has been detected in the effluent of a chemical specialties manufacturing plant (0.01-0.30 ppm) (2), iron and steel manufacturing (53 ppm maximum), leather tanning and finishing (1.4 ppm maximum), aluminum forming (9.7 ppm maximum), electrical/electronic component manufacturing (3.5 ppm maximum), foundries, (34 ppm maximum), pharmaceuticals (4.6 ppm maximum), organics/plastics manufacturing, and paint and ink formulating (1.2 ppm maximum), and rubber processing operations (12 ppm maximum) (3). It has also been detected in quench water from a coking operation (4), discharges from coal gassification plants (5), industrial and municipal landfill leachate (6), refinery effluent (7), and municipal wastewater sludge incineration (8, 9).

General population exposure to phenol may occur through inhalation as it has been detected in ambient air samples in urban, suburban, and source dominated areas (10-12), as well as in automobile exhaust and tobacco smoke (13). The presence of phenol in drinking water supplies (14) and ground water after spills (15) may also lead to general population exposure through the ingestion of contaminated water.

[(1) U.S. EPA; Toxics Release Inventory (1992) (2) Jungclaus GA et al; Environ Sci Tech 12: 88-96 (1978) (3) U.S. EPA; Treatability Manual p. I.8.1-3 EPA-600/2-82-001A (1981) (4) O'Malley MA; Health Hazard Evaluation Report No.

HETA-85-441-1765, New Boston Coke Corporation, New Boston, OH. Hazard Evaluations and Technical Assistance Branch, NIOSH, U.S. Department of Health and Human Services, Cincinnati, OH (1986) (5) Bombaugh KJ, Rhodes WJ; Environ Sci Technol 22: 1389-96 (1988) (6) Brown KW, Donnelly KC; Haz Waste Haz Mat 5: 1-26 (1988) (7) Cardwell TJ et al; Intern J Environ Anal Chem 24: 23-35 (1986) (8) DeWees WG et al; Emissions of Metals, Chromium and Nickel Species, and Organics from Municipal Wastewater Sludge Incinerators. EPA/600/SR-92/003 EPA Risk Reduction Engineering Lab, Cincinnati, OH (1992) (9) Vancil MA et al.; Emissions of Metals and Organics from Municipal Wastewater Sludge Incinerators. EPA/600/S2-91/007 EPA Risk Reduction Engineering Lab, Cincinnati, OH (1991) (10) Brodzinsky R, Singh HB; Volatile Organic Compounds in the Atmosphere: An Assessment of Available Data. SRI International. EPA Contract 68-02-3452 (1982) (11) Hoff RM, Chan KW; Environ Sci Technol 21: 556-61 (1987) (12) Scow K et al; Exposure and Risk Assessment for Phenol (Revised) p. 76 EPA/440/4-85/013 (1981) (13) Graedel TE; Chemical Compounds in the Atmosphere p. 256 New York, NY: Academic Press Inc (1978) (14) Nicola RM; J Environ Health 49: 342-7 (1987) (15) Delfino JJ, Dube DJ; J Environ Sci Health A11: 345-55 (1976)]

Environmental Transport and Persistence:

Bioaccumulation: Experimental bioconcentration factors for phenol are 1.9 for goldfish (*Carassius auratus*) (1), 277 for water flea (*Daphnia magna*) (2), 20 for goldfish (3), 200 for algae (*Clorella fusca*) (3), and 3.5 for freshwater phytoplankton (*Scenedesmus quadricauda*) (4). These values indicate that phenol will not significantly bioconcentrate in fish and aquatic organisms.

[(1) Kobayashi K et al; Bull Jap Soc Sci Fish 45: 173-5 (1979) (2) Dauble DD et al; Bull Environ Contam Toxicol 37: 125-32 (1986) (3) Freitag D et al; p. 119 In: QSAR Environ Toxicol Proc Workshop Quant Struct-Act Relat. Kaiser KLE ed Reidel: Netherlands (1984) (4) Hardy JT et al; Environ Toxicol Chem 4: 29-35 (1985)]

Volatilization/Adsorption: According to a simple fugacity model, the mass distribution of phenol among the environmental compartments at equilibrium is 55% to water, 45% to air, and none to soil (1). The Henry's Law constant for phenol indicates that it will volatilize from water to air at a rate slower than that for water itself (2). Similarly, its volatilization from moist soil to the atmosphere will be slow. However, its vapor pressure indicates that volatilization from dry soil may be relatively rapid.

Experimental soil adsorption coefficients obtained using a wide variety of soil types ranged from 16 to 91 (3-6). This indicates that phenol will display high to very high mobility in soil (7). Other workers have observed little to no adsorption of phenol to clay soils, silt loams, and aquifer material (8, 9). Despite its high solubility and expected mobility, biodegradation of phenol is sufficiently rapid that groundwater is generally free of this compound (9). Phenol is a weak acid and partially dissociated in neutral and basic soils and thus, its movement through soil is governed by its water solubility; it may be more strongly adsorbed in acidic soils (10) and some clay soils (11).

(1) U.S. EPA; PCGEMS (Graphical Exposure Modeling System), PCENPART (Environmental Partitioning Model) (2) Lyman WJ et al; Handbook of Chemical Property Estimation Methods. Environmental Behavior of Organic Compounds New York, NY: McGraw-Hill p. 4-9 (Eqn 4-5), 15.1-15.34 (1982) (3) Kenaga EE; Ecotoxicol Environ Safety 4: 26-38 (1980) (4) Boyd SA (1982) (5) Briggs GG; Aust J Soil Res 19: 61-8 (1981) (6) Scott HD et al; J Environ Qual 12: 91-5 (1983) (7) Swann RL et al; Res Rev 85: 17-28 (1983) (8) Artioli-Fortuny J, Fuller WH; Soil Sci 133: 18-26 (1982) (9) Ehrlich GG et al; Groundwater 20: 703-10 (1982)

(10) Laquer FC, Manahan SE; Chemosphere 16: 1431-45 (1987) (11) Stockmeyer MR; Appl Clay Sci 6: 39-57 (1991)]

Persistence: Phenol is a benchmark chemical for biodegradability studies and there is a large body of information on its degradation, which concludes that phenol rapidly degrades in sewage, soil, freshwater, and seawater (1-8). Biodegradation is generally rapid with complete removal occurring in a matter of days (1-3). Acclimation of resident populations of microorganisms is also rapid. Under anaerobic conditions degradation is slower and microbial adaptation periods longer (1) although complete degradation has been found to occur (9, 10). The exception to the biodegradation of phenol in the environment would be in the cases of spills where high concentrations (>100 mg/L) of phenol destroy degrading microbial populations (11-13).

In the upper layers of sunlit natural water, phenol is susceptible to relatively rapid degradation via the reaction with photochemically produced hydroxyl and alkylperoxy radicals. Typical half-lives for these processes are on the order of 100 and 19.2 hours of sunlight, respectively (14).

The gas/particle partitioning of semivolatile organic compounds in the atmosphere depends on the vapor pressure of the organic compound and the concentration of total suspended particulate matter (15). According to this theory, atmospheric phenol will be primarily found in the vapor phase and is subject to relatively rapid oxidative degradation. An experimental rate constant for the gas-phase reaction of phenol with photochemically produced hydroxyl radicals of $2.63 \times 10^{11} \text{ cm}^3/\text{molecule-sec}$ (16) translates to a half-life of 21 hours (of sunlight) using an average atmospheric hydroxyl radical concentration of $5 \times 10^5 \text{ molecules/cm}^3$. Similarly, the night-time reaction of phenol with nitrate radicals has a half-life of 15 minutes based on a rate constant of $3.8 \times 10^{12} \text{ cm}^3/\text{molecule-sec}$ (17).

(1) Baker MD, Mayfield CI; Water Air Soil Pollut 13: 411 (1980) (2) Ehrlich GG et al; Groundwater 20: 703-10 (1982) (3) Healy JB, Young LY; Food Microbiol Toxicol 38: 84-9 (1978) (4) Arvin, E; Org Micropollut Aquat Environ. Proc Eur Symp 6th pp. 174-8 (1991) (5) Brown SC et al.; Wat Res 24: 853-61 (1990) (6) Kirk PWW, Lester JN; Environ Tech Lett 10: 404-14 (1989) (7) Kuiper J, Hanstveit HA; Biodegradation Rates of Xenobiotic Compounds in Plankton. Oceanic Processes in Marine Communities Volume 1. Malabar, FL: Robert E. Krieger Publishing Co pp. 79-87 (1988) (8) Bhattacharya SK et al.; Removal and Fate of RCRA and CERCLA Toxic Organic Pollutants in Wastewater Treatment. EPA/600/S2-89/026 EPA Risk Reduction Engineering Lab, Cincinnati, OH (1990) (9) Battersby NS, Wilson V; Appl Environ Microbiol 55:433-9 (1989) (10) Godsy EM et al.; Biodegradation 2: 211-21 (1992) (11) Delfino JJ, Dube DJ; J Environ Sci Health A11: 345-55 (1976) (12) Gerike P, Gode, P; Chemosphere 21: 799-812 (1990) (13) O'Connor OA, Young LY; Environ Toxicol Chem 8: 853-62 (1989) (14) Mill T et al; Science 207: 886-7 (1982) (15) Eisenreich SJ et al; Environ Sci Technol 15: 30-8 (1981) (16) Atkinson R; Chem Rev 85: 69-201 (1985) (17) Atkinson R et al; Environ Sci Technol 21: 1123-6 (1987)]

DIETHANOLAMINE

SUBSTANCE IDENTIFICATION

Synonyms: DEA; 2,2'-iminodiethanol; 2,2'-dihydroxydiethylamine; bis(2-hydroxyethyl)amine
Structure:



CAS Registry Number: 111-42-2

Molecular Formula: C₄H₁₁O₂N

CHEMICAL AND PHYSICAL PROPERTIES

Boiling Point: 268.8 °C decomposes

Melting Point: 28 °C

Molecular Weight: 105.14

Dissociation Constants: 8.88 (2)

Log Octanol/Water Partition Coefficient (log K_{ow}): -1.43 (1)

Water Solubility: 95.4% (weight) (2)

Vapor Pressure: 2 x 10⁻⁴ mm Hg @ 20 °C (2)

Henry's Law Constant: 5.35 x 10⁻¹⁴ atm·m³/mole (3)

Lower Explosive Limit: Not available

[(1) Hansch C, Leo AJ; Medchem Project Issue No 26 Claremont, CA: Pomona College (1985) (2) Riddick JA et al; Organic Solvents 4th ed; p. 705 New York, NY: Wiley (1986) (3) Hine J, Mookerjee PK; J Org Chem 40: 292-8 (1975)]

EXPOSURE PROFILE

Production: The U.S. ITC reports diethanolamine (DEA) sales of 166 million pounds for 1991, out of a production of 198 million pounds (1). *Ethanolamines* are produced by Union Carbide (Seadrift, TX), Texaco (Port Neches, TX), Dow (Plaquimine, LA and Midland, MI), and Occidental Petroleum (Bayport, TX) (2). In 1991, 36% of *ethanolamine* production (mono-, di-, and triethanolamine) was exported (3).

[(1) USITC; Synthetic Organic Chemicals. United States Production and Sales, 1991. USITC Publication 2607. p. 15-4 February 1993 (2) SRI International; 1993 Directory of Chemical Producers, United States of America p. 590 (1993) (3) Chemical Marketing Reporter; Chemical Profile: Ethanolamines. September 28, 1992]

Use: Diethanolamine is used as a chemical intermediate in the production of surfactants, personal care products such as creams, lotions, shampoos, soaps and cosmetics, and detergents (2, 3). It is

used in adhesives, cleaners, coatings, corrosion inhibitors for ferrous metals in applications such as coolant systems, lubricating oils, metal working fluids, petroleum antifouling and drilling, and electroplating baths (2). It is used for "sweetening" natural gas and neutralizing acid herbicides (2). DEA or its derivatives are also used in many facets of textile production (2). The use pattern for *ethanolamines* are surfactants (40%), gas purification (25%), metals (17%), textiles (8%), and other, including cement grinding oils and agricultural chemicals (10%) (1). Alkanolamine-based surfactants are generally *alkanolamides* (nonionic surfactants) and *alkanolamine salts* (anionic surfactants) (2).

[(1) Chemical Marketing Reporter; Chemical Profile: Ethanolamines. September 28, 1992 (2) Bollmeier AF Jr; Kirk-Othmer Encyclopedia of Chemical Technology, 4th ed. 2: 1-34 (1992) (3) Cahn A, Lynn JL Jr; Kirk-Othmer Encyclopedia of Chemical Technology, 3rd ed. 22: 373-374 (1983)]

Occupational Exposure: NIOSH (NOES Survey 1981-83) has statistically estimated that 573,025 workers are exposed to DEA in the United States (1). According to the 1991 TRI, 144 reporting user sites either repackaged DEA or used it as a formulating agent (8), so that DEA is sent off-site to other companies and/or consumers. There were 242 reporting user sites that consumed DEA (8) on-site where potential occupational exposure to DEA was limited to the site. DEA is used in the formulation of acidic herbicides such as Dinoseb (3) and workers who are engaged in formulating and applying these herbicides may be exposed to DEA. The presence of N-nitrosodiethanolamine is an indicator of DEA (see Persistence below). On the basis of N-nitrosodiethanolamine detection, 14 of 18 metal-working fluids recently obtained from American manufacturers contained DEA (4). Workers may be exposed to DEA by inhalation and dermal contact during the use of lubricating liquids in various processes in machine building and metallurgy (cutting, die stamping, grinding, extrusion, die casting, etc.) (2, 4). In a 1977-1981 NIOSH study of N-nitrosamines in manufacturing facilities, a factory using cutting fluids had 0.08 $\mu\text{g}/\text{m}^3$ of *N-nitrosodiethanolamine* (5, 6). Similar results were obtained from a survey of commercially obtained cutting fluids (7). DEA, *itself*, has been detected at a concentration of 0.25 to 0.40 mg/m^3 in the air of a workroom in Russia where automobile engine parts were being processed (2).

[(1) NIOSH. National Institute for Occupational Safety and Health. National Occupational Exposure Survey (NOES). Computer printout March 29, 1989 (2) Berezkin VG, Drugov S; Zavod Lab 52: 16-9 (1986) (3) Wigfield YY et al; J Assoc Anal Chem 70: 792-796 (1987) (4) Keefer LK et al; Food Chem Toxicol 28: 531-534 (1990) (5) Fajen JM et al; Summary report of N-nitrosamines in the factory environment. IARC Sci Publ No. 41: 223-229 (1982) (6) Fan S, Fajen J; Survey for N-nitroso compounds at Chrysler Forge and Axle Plant, Detroit Michigan. NIOSH 00122556 Cincinnati, OH: NIOSH NTIS PB 3 153767 (1978) (7) Williams DT et al; Bull Environ Contam Toxicol 20: 206-211 (1978) (8) U.S. EPA; Toxics Release Inventory (1992)]

Consumer Exposure: No information was found concerning consumer exposure to DEA. While DEA is used for making consumer products such as detergents and personal care products, derivatives of DEA, *and not DEA itself*, are often present in these products (1, 2). The presence of N-nitrosodiethanolamine is an indicator of DEA (see Persistence below). On the basis of N-

nitrosodiethanolamine detection, DEA may have been present in all seven cosmetics, fourteen lotions, and ten shampoos obtained in the Boston area and tested for N-nitrosodiethanolamine (3)

[(1) Isacoff H; Kirk-Othmer Encyclopedia of Chemical Technology, 2nd ed. 7: 143-176 (1979) (2) Bollmeier AF Jr; Kirk-Othmer Encyclopedia of Chemical Technology, 4th ed. 2: 1-34 (1992) (3) Fan TY et al; Food Cosmet Toxicol 15: 423-430 (1977)]

Environmental Release and General Population Exposure: According to the 1991 Toxics Release Inventory (TRI), 897,752 pounds of DEA were released to the environment, of which 48.3% was released to water, 30.2% into the atmosphere, and 14.8% to land (1). No data were found on levels of DEA in environmental media. DEA was not reported in effluent from any of the 4,000 industrial and publicly owned treatment works (POTWs) surveyed by the Effluent Guidelines Division of EPA (2).

The presence of N-nitrosodiethanolamine is an indicator of DEA (see Persistence below). On the basis of N-nitrosodiethanolamine detection, the general population may be exposed to DEA from tobacco, tobacco smoke, and snuff (3).

[(1) U.S. EPA; Toxics Release Inventory (1992) (2) Shackelford WM et al; Analyt Chim Acta 146: 15-27 (supplemental data) (1983) (3) Preussmann R; Occurrence and exposure to N-nitroso compounds and precursors. IARC Science Publication No. 57: 3-15 (1984)]

Environmental Transport and Persistence:

Bioaccumulation: The very high solubility of DEA in water indicates that it should not bioconcentrate in aquatic organisms (1).

[(1) Lyman WJ et al; Handbook of Chemical Property Estimation Methods NY: McGraw-Hill p. 5-5 (1982)]

Volatilization/ Adsorption: According to a simple fugacity model, DEA will distribute entirely to water (1). Its very low Henry's Law constant indicates that it will not volatilize from surface waters (2). The pK_a value for DEA indicates that it will be almost entirely dissociated at environmental pHs. The very high solubility of DEA indicates that this chemical will be extremely mobile in soil and not adsorb appreciably to organic matter in aqueous suspended solids and sediment (2); the fact that DEA is protonated in water may result in greater adsorption and less mobility than its water solubility would predict because such estimations do not include ionic interactions. DEA has been shown to adsorb (40-45%) to humic acids, which may be contained in soils and sediments (3). The adsorption of DEA to humic acids changes very slightly from pH 4 to 8 (3).

[(1) U.S. EPA; PCGEMS (Graphical Exposure Modeling System), PCENPART (Environmental Partitioning Model) (2) Lyman WJ et al; Handbook of Chemical Property Estimation Methods NY: McGraw-Hill, pp. 4-1 to 4-33, 15-1 to 15-34 (1982) (3) Sithole BB, Guy RD; Environ Int 11: 499-504 (1985)]

Persistence: In the atmosphere, DEA will exist primarily in the vapor phase (2). As a vapor, it reacts with photochemically-produced hydroxyl radicals in the atmosphere with a rate constant of $1.03 \times 10^{-10} \text{ cm}^3/\text{molecule-s}$ (1). Assuming a hydroxyl radical concentration of $5 \times 10^5 \text{ radicals/cm}^3$, the half life of DEA in the atmosphere is 3.7 hours. DEA is a base with a pK_a of 8.88 and will exist almost entirely as a cation at neutral pHs; only above pH 8 will a substantial percentage (>10%) of DEA be undissociated. DEA is readily nitrosated to N-nitrosodiethanolamine in the presence of nitrous acid, nitrites, or oxides of nitrogen (13, 14). This reaction may even occur during stirring or mild heating (14). (Under suitable conditions, triethanolamine (TEA) can be similarly nitrosated to N-nitrosodiethanolamine (13, 14)). The detection of N-nitrosodiethanolamine indicates that DEA, or possibly TEA, and a suitable nitrosating agent are present. The situation is further complicated by the fact that commercial TEA contains DEA *as an impurity* (15).

DEA is readily biodegraded and mineralized according to a large number and variety of laboratory tests using activated sludge and wastewater inocula (4-12). In a 4-day die-away test in stream water, 5%, 55%, and 32% of DEA was mineralized for initial concentrations of 21 mg/L, 210 µg/L, and 21 ng/L, respectively (3). In Cayuga Lake and North Lake (acidic) water, 31% and 1.2% mineralization occurred in 14 days, respectively (4). N-Nitrosodiethanolamine has been identified as a metabolite of DEA in natural water samples and sewage (4)

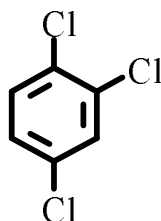
[(1) Atkinson R; J Phys Chem Ref Data. Monograph 1 pp. 188, 195 (1989) (2) Bidleman T; Environ Sci Technol 22: 361-367 (1988) (3) Boethling RS, Alexander M; Environ Sci Tech 13: 989-91 (1979) (4) Yordy JR, Alexander M; J Environ Qual 10: 266-70 (1981) (5) Kitano M; OECD Tokyo Meeting Reference Book Tsu-No. 3 (1978) (6) Mills EJ, Stack VT; Proc 9th Ind Waste Conf Eng Bull Purdue Univ: Ext Ser 9: 449-64 (1955) (7) Lamb CB, Jenkins GF; pp. 326-39 in Proc 8th Ind Waste Conf Purdue Univ (1952) (8) Price KS et al; J Water Poll Contr Fed 46: 63-77 (1974) (9) Bridie AL et al; Water Res 13: 627-30 (1979) (10) Gannon JE et al; Microbios 23: 7-18 (1978) (11) Pitter P; Water Res 10: 231-235 (1976) (12) Gerike P, Fischer WK; Ecotoxicol Environ Safety 3: 159-73 (1979) (13) Hammer H; Ullmann's Encyclopedia of Industrial Chemistry A10: 1-6 (1987) (14) Fan TY et al; Food Cosmet Toxicol 15: 423-430 (1977) (15) Fan S, Fajen J; Survey for N-nitroso compounds at Chrysler Forge and Axle Plant, Detroit Michigan. NIOSH 00122556 Cincinnati, OH: NIOSH NTIS PB 3 153767 (1978)]

1,2,4-TRICHLOROBENZENE

SUBSTANCE IDENTIFICATION

Synonyms: *unsym*-Trichlorobenzene

Structure:



CAS Registry Number: 120-82-1

Molecular Formula: C₆H₃Cl₃

CHEMICAL AND PHYSICAL PROPERTIES

Boiling Point: 213.5 °C

Melting Point: 17 °C

Molecular Weight: 181.46

Dissociation Constants: Not applicable

Log Octanol/Water Partition Coefficient (log K_{ow}): 4.02 (1)

Water Solubility: 48.8 mg/L @ 20 °C (2)

Vapor Pressure: 0.29 mm Hg @ 25 °C (3)

Henry's Law Constant: 1.42 x 10⁻³ atm-m³/mole (calculated from the vapor pressure and water solubility)

Lower Explosive Limit: Not available

[(1) Hansch C, Leo AJ; Medchem Project Issue No 26 Claremont, CA: Pomona College (1985) (2) Chiou PE et al; Environ Sci Technol 17: 227-31 (1983) (3) U.S. EPA; Ambient Water Quality Criteria: Chlorinated Benzenes p. C-34. EPA 440/5-80-028 (1980)]

EXPOSURE PROFILE

Production: No non-CBI production information is available for 1,2,4-trichlorobenzene. 1,2,4-Trichlorobenzene is produced by Standard Chlorine of Delaware (Delaware City, DE) (1, 2), where it is both sold and used as a formulating ingredient (3). All chlorobenzenes are presently produced by the catalytic chlorination of benzene, an *ortho*-, *para*-directed reaction. Therefore, 1,2,4-trichlorobenzene may be produced as a byproduct or an impurity in the production of large production chemicals such as monochlorobenzene, *o*-dichlorobenzene, and *p*-dichlorobenzene.

According to the 1991 Toxic Chemical Release Inventory (TRI) submissions, there are 11 facilities that manufacture *or* import 1,2,4-trichlorobenzene, 9 facilities that manufacture 1,2,4-trichlorobenzene, and 3 facilities that import 1,2,4-trichlorobenzene (3). The additional producers of 1,2,4-trichlorobenzene are: PPG Industries (Westlake, LA and New Martinsville, WV) which produces it as a byproduct and for sale; Vista Chemical Co. (Westlake, LA) which produces it as a byproduct; Occidental Chemical Corporation (Deer Park, TX) which produces it as a byproduct; Piedmont Chemical Industries (High Point, NC) which imports it for on-site use as a formulating ingredient; Sandoz Agro Inc. (Beaumont, TX) which imports it for on-site use as a reactant; Virkler Co. (Charlotte, NC) which produces it for sale and uses it as a formulating ingredient; Sun Refining and Marketing Co. (Marcus Hook, PA) which produces and imports chemicals in which it is an impurity; Weslake Monomers Corporation (Calvert City, KY) which produces it for on-site use as a reactant; and Monsanto Co. (Sauget, IL) which produces it as a byproduct. Standard Chlorine of Delaware (Delaware City, DE) and PPG Industries (New Martinsville, WV) produce 1,2,4-trichlorobenzene for sales and distribution but annual production volumes are not available. The maximum amount stored on site at these two facilities combined, based on Toxics Release Inventory submissions, is between 1.1 and 11 million pounds (3).

[(1) SRI International; 1993 Directory of Chemical Producers, United States of America p. 989 (1993) (2) USITC; Synthetic Organic Chemicals. United States Production and Sales, 1991. USITC Publication 2607. p. 3-11. February 1993 (3) U.S. EPA; Toxics Release Inventory (1992)]

Use: *Trichlorobenzenes* are used in some pesticides, as a dye carrier, in dielectric fluids, in lubricants, as a heat-transfer medium, and as an organic intermediate and solvent used in chemical manufacturing (2); however, the market for these uses is small and declining (2). Of the trichlorobenzenes, only 1,2,4-trichlorobenzene and 1,2,3-trichlorobenzene are sold in larger than research quantities (3). Dye carriers are used in the textile industry to achieve complete dye penetration of polyester fibers (4). They loosen the interpolymer dyes and allow water insoluble dyes to penetrate into the fiber. Trichlorobenzenes are one of the most commonly used dye carriers (4). 1,2,4-Trichlorobenzene was one of the most frequently used solvents in a gallium-arsenide wafer fabrication facility employing about 70 workers (1).

[(1) Lenihan KL; Preliminary survey report: Control technology for gallium arsenide processing at Honeywell, Inc., Richardson, Texas, Report No. CT-163-17A. NIOSH/00177544. NIOSH, Cincinnati, OH (1987) (2) Bryant JG; Kirk-Othmer Encyclopedia of Chemical Technology, 4th ed. 6: 87-100 (1993) (3) Chemyclopedia93; American Chemical Society volume 11, p.117 (1992) (4) Wannmacher R, DeMaria; Kirk-Othmer Encyclopedia of Chemical Technology, 3rd ed. 8: 151-158 (1979)]

Occupational Exposure: NIOSH (NOES Survey 1981-83) has statistically estimated that 4,032 workers are exposed to 1,2,4-trichlorobenzene in the United States (1).

No occupational exposure levels were found for 1,2,4-trichlorobenzene. Occupational exposure to 1,2,4-trichlorobenzene may occur from inhalation or dermal contact in industries that produce 1,2,4-trichlorobenzene or use it as a dye carrier (e.g., textile industry), solvent (e.g., wafer fabrication), etc.

[(1) NIOSH. National Institute for Occupational Safety and Health. National Occupational Exposure Survey (NOES). Computer printout March 29, 1989]

Consumer Exposure: No consumer products containing 1,2,4-trichlorobenzene were identified.

Environmental Release and General Population Exposure: According to the 1991 Toxics Release Inventory (TRI), 419,025 pounds of 1,2,4-trichlorobenzene were released to the environment, of which 98% was released into the atmosphere (1). Most of 528,594 pounds of 1,2,4-trichlorobenzene waste that was transferred off site was incinerated (1). A reasonable worst case estimate of annual 1,2,4-trichlorobenzene stack emissions from hazardous waste incinerators is 1,340 pounds (4). 1,2,4-Trichlorobenzene was found in fly ash of 2 municipal incinerators at 81 and 250 ppb; fly ash or combined ash from six other incinerators did not contain detectable levels of 1,2,4-trichlorobenzene (20). 1,2,4-Trichlorobenzene is formed in the thermal decomposition of polyvinylidene chloride (23). Raw effluent from a textile plant in the southeastern U.S. that primarily finished polyester fabrics contained the dye carrier 1,2,4-trichlorobenzene (3).

In a comprehensive survey of wastewater from 4,000 industrial and publicly owned treatment works (POTWs) sponsored by the Effluent Guidelines Division of the U.S. EPA, 1,2,4-trichlorobenzene was identified in discharges of the following industrial category (positive occurrences; median concentration in ppb): printing and publishing (4; 40.9), organics and plastics (1; 178.5), inorganic chemicals (1; 2.3), textile mills (4; 277.2), plastics and synthetics (1; 76.8), auto and other laundries (1; 9.7), pesticides manufacture (2; 197.9), electronics (2; 51.8), organic chemicals (33; 33.7), and POTWs (42; 44.4) (2). The highest effluent concentration was 1,854 ppb in a POTW, followed by 1,350 ppb in the organic chemicals industry (2).

Atmospheric 1,2,4-trichlorobenzene concentrations in Los Angeles, Phoenix, and Oakland, in 1979, were 19.7 to 339.4 ppt, 8.7 to 101.5 ppt, and 8.7 to 101.5 ppt, respectively; mean levels ranged from 29.5 to 69.3 ppt (15). The concentration of 1,2,4-trichlorobenzene in air during seven rain events in Portland, OR was 3.4 to 4.7 ng/m³ (12). The corresponding concentration of 1,2,4-trichlorobenzene in rain was 0.13 to 0.45 ng/L for three of the event and below the detection limit for the other four events. A study of indoor air pollutants in 300 Dutch homes in 2 cities between 1981 and 1983, found that the maximum concentrations of 1,2,4-trichlorobenzene indoors and outdoors were 33 and <0.8 µg/m³ (17). While the source of the 1,2,4-trichlorobenzene in the homes was not established, cleaning agents, pesticides, and building materials may release chlorobenzenes (17).

A 1976-77 study of drinking water in 11 cities of the U.S. (110 samples) found that 91% of the samples contained 1,2,4-trichlorobenzene levels between 0.01 and 0.53 ppb, with a mean of 0.09 ppb (9).

During 1983, the concentration of 1,2,4-trichlorobenzene ranged from 0.022 to 1.360 ng/L at fourteen stations in Lake Ontario that were sampled for organochlorine contaminants. The highest value was in a station near Niagara Falls which also had very high concentrations of other

chlorinated benzenes (16). From 1981 to 1983, the concentration of 1,2,4-trichlorobenzene in the Niagara River at Niagara-on-the-Lake (104 samples) ranged from 5.8 to 120 ng/L with a mean of 16 ng/L (18). In 1980, 1,2,4-trichlorobenzene concentrations in sections of the Great Lakes were: Lake Ontario (5 stations), 0.3 to 1 ng/L with a mean of 0.6 ng/L; Lake Huron, 0.1 to 0.4 ng/L with a mean of 0.2 ng/L; Grand River, Ontario, ND to 8 ng/L with a mean of 2 ng/L; and Niagara River (4 stations), 0.1 to 107 ng/L (5). On the Niagara River, the station with the highest 1,2,4-trichlorobenzene level was just below chemical manufacturer's effluent discharge; the mean level at the other three stations was 6.4 ng/L (6).

The median and maximum 1,2,4-trichlorobenzene concentration in the North Sea (Rhine/ Meuse Estuary) between August 1983 and July 1984 was 1.0 and 24 ppt, respectively (10).

The maximum concentration of 1,2,4-trichlorobenzene in rain measured during 16 rain events between 1982 and 1984 was 0.45 ppt; 1,2,4-trichlorobenzene was not detected in 10 of the rain events (11, 12).

The highest mean levels of 1,2,4-trichlorobenzene in sediment from EPA's STORET database for 1978 to 1987 were from the East South Central region of the U.S. (13); the lowest were from New England (13). The mean concentrations of 1,2,4-trichlorobenzene in sediment from Southern Lake Huron, Lake St. Clair, Western Lake Erie, Central Lake Erie, and Eastern Lake Erie were 2.4, 4.3, 2.1, 5.3, 2.3, and 2.4 ppm (dry weight), respectively (14). The maximum concentration, 14 ppm, was found in Western Lake Erie (14).

In a 1980 study, trout from five sites in the Great Lakes trout contained between 0.5 and 5 ppb of 1,2,4-trichlorobenzene (6). Ten rainbow trout taken from Lake Ontario in 1983 contained a mean 1,2,4-trichlorobenzene concentration of 0.6 ppb (8). Livers of flatfish collected from four sites near a Southern California municipal wastewater outfalls contained average 1,2,4-trichlorobenzene levels of <3.4 to 26 ppb, whereas it was not detected at a control site (7). The highest mean levels of 1,2,4-trichlorobenzene in fish tissue from EPA's STORET database for 1978 to 1987 were from the East North Central region of the U.S. (13).

Herring gull eggs collected near the Detroit and Niagara Rivers in 1979 all contained 1,2,4-trichlorobenzene and had average 1,2,4-trichlorobenzene concentrations of 0.01 ppm and 0.02 ppm, respectively (5).

The estimated yearly intake of 1,2,4-trichlorobenzene from the diet is 62.3 µg of which 71.3% comes from eggs and meat and 19.6% from leafy vegetables (22).

The concentrations of 1,2,4-trichlorobenzene in whole breast milk and milk fat, according to a Canadian national survey, were 0.6 and 64 ppb, respectively (19). The corresponding values for a sample of eighteen indigenous Canadian women were 1.2 and 64 ppb (19). Indigenous women generally eat a greater quantity of fish and meat than the general population. The mean and

maximum concentrations of 1,2,4-trichlorobenzene in adipose fat according to a 1985 Canadian survey were 103 and 358 ppb, respectively; 26% of specimens contained detectable residues (21).

[(1) U.S. EPA; Toxics Release Inventory (1992) (2) Shackelford WM et al; *Analyt Chim Acta* 146: 15-27 (supplemental data) (1983) (3) Gordon AW, Gordon M; *Trans KY Acad Sci* 42: 149-57 (1981) (4) Dempsey CR; *J Air Waste Manage Assoc* 43: 1374-1379 (1993) (5) Struger J et al; *J Great Lakes Res* 11: 223-30 (1985) (6) Oliver BG, Nicol KD; *Environ Sci Technol* 16: 532-6 (1982) (7) Young DR et al; In: *Water Chlorination Environmental Impact and Health Effects* 3: 471-86 (1980) (8) Oliver BG, Niimi AJ; *Environ Sci Technol* 19: 842-9 (1985) (9) McNamara PW et al; *Exposure and risk assessment for 1,2,4-trichlorobenzene* EPA-440/4-85-017 (1981) (10) VandeMeent D et al; *Water Sci Technol* 18: 73-81 (1986) (11) Pankow JF et al; *Environ Sci Technol* 18: 310-8 (1984) (12) Ligocki MP et al; *Atmos Environ* 19: 1609-17 (1985) (13) Phillips LJ et al; *Chemosphere* 22: 835-848 (1991) (14) Oliver BG, Bourbonniere RA; *J Great Lakes Res* 11: 366-72 (1985) (15) Singh HB et al; *Atmospheric measurements of selected toxic organic chemicals* PB80-19889 (1980) (16) Biberhofer J, Stevens, RJJ; *Organochlorine contaminants in ambient waters of Lake Ontario. Scientific Series No. 159* Burlington, Ontario: Inland Waters/Lands Directorate (1987) (17) Otson R, Fellin P; *Gaseous Pollutants: Characterization and Cycling*, JO Nriagu, Ed. pp. 335-421 John Wiley & Sons (1992) (18) Oliver BG, Nicol KD; *Sci Tot Environ* 39: 57-70 (1984) (19) Davies D, Mes J; *Bull Environ Contam Toxicol* 39: 743-750 (1987) (20) Shane BSS et al; *Arch Environ Contam Toxicol* 19: 665-673 (1990) (21) Mes J et al; *Bull Environ Contam Toxicol* 45: 681-688 (1990) (23) Davies K; *Chemosphere* 17: 263-276 (1988) (22) Yashuhara A, Morita M; *Environ Sci Technol* 22: 646-650 (1988)]

Environmental Transport and Persistence:

Bioaccumulation: The bioconcentration factors (BCFs) for 1,2,4-trichlorobenzene in fish are 2,800 in Fathead minnow (1), 1,300 in Rainbow trout (2); 124 to 1,300 in eight species of fish, with a mean of 863 (3), 812 in Bluegill sunfish (4), and 490 in Golden ide (*Leuciscus idus melanotus*) (5). The BCF of 1,2,4-trichlorobenzene in juvenile American flagfish (*Jordanella floridae*) determined in a 28-day study was 2,026 (6). These BCFs indicate that 1,2,4-trichlorobenzene has a moderate to high potential for accumulating in aquatic organisms. The uptake time required to reach 90% steady state was 4.03 days, while the depuration half-life was 1.21 days (6).

[(1) Veith GD et al; *J Fish Res Board Can* 36: 1040-8 (1979) (2) Oliver BG, Niimi AJ; *Environ Sci Technol* 19: 842-8 (1985) (3) Geyer H et al; *Chemosphere* 14: 545-55 (1985) (4) Barrows ME et al; pp. 379-92 in *Dynamic Exposure and Hazard Assessment of Toxic Chemicals* Ann Arbor, MI: Ann Arbor Sci (1980) (5) Freitag D et al; *Chemosphere* 14: 1589-1616 (1985) (6) Smith AD et al; *Chemosphere* 20: 379-386 (1990)]

Volatilization/ Adsorption: According to a simple fugacity model, the mass distribution of 1,2,4-trichlorobenzene among the environmental compartments at equilibrium will be almost entirely (99.99%) to air (1). Using its Henry's Law constant, the volatilization half-life for 1,2,4-trichlorobenzene in a 1 m deep model river with a 1 m/s current and a 3 m/s wind speed is 4.8 hours (2). Similarly, the volatilization half-life for 1,2,4-trichlorobenzene from a 1 m deep model lake with a 0.05 m/s current and a 0.5 m/s wind is 5.6 days (2). The volatilization half-lives of 1,2,4-trichlorobenzene determined in a 5.4 m-deep seawater mesocosm that was mixed four times a day to simulate waves with temperature and initial 1,2,4-trichlorobenzene concentration adjusted to simulate seasonal conditions in Narragansett Bay, RI were: Spring (8-16 °C, 0.5 ppb), 22 days; Summer (20-22 °C, 0.2 ppb), 11 days; and Winter (3-7 °C, 2.2 ppb), 12 days (3).

K_{oc} values that have been reported for 1,2,4-trichlorobenzene include: 1,441 in a peaty soil (4); 872 in a silt loam soil (5); and 1,000 in a fine sand soil (6). 1,2,4-Trichlorobenzene was significantly retarded in the fine sand soil; the retardation factor was 9.4 (6). The K_{oc} for 1,2,4-trichlorobenzene estimated from its water solubility is 514 (2) and that estimated from structure-activity relations is 718 (7). These results indicate that 1,2,4-trichlorobenzene has a low mobility in soil (8). 1,2,4-Trichlorobenzene that was injected into a confined aquifer was not detected in observation wells (9). Assuming its behavior is similar to that of dichlorobenzenes, the fact that 1,2,4-trichlorobenzene was not detected is because of its effective adsorption by aquifer material, rather than biodegradation (9).

[(1) U.S. EPA; PCGEMS (Graphical Exposure Modeling System), PCENPART (Environmental Partitioning Model) (2) Lyman WJ et al; Handbook of Chem Property Estimation Methods Environ Behavior of Org Compounds McGraw-Hill NY pp. 4-9 (Eqn 4-6), 15-1 to 15-34 (1982) (3) Wakeham SG et al; Environ Sci Technol 17: 611-17 (1983) (4) Friesel P et al; Fresenius Z Anal Chem 319: 160-4 (1984) (5) Chiou CT et al; Environ Sci Technol 17: 227-31 (1983) (6) Wilson JT et al; J Environ Qual 10: 501-6 (1981) (7) Meylan WM et al; Environ Sci Technol 26: 1560-7 (1992) (8) Swann RL et al; Res Rev 85: 17-28 (1983) (9) Roberts PV et al; J Water Pollut Control Fed 52: 161-72 (1980)]

Persistence: 1,2,4-Trichlorobenzene does not hydrolyze significantly under environmental conditions (1). The hydrolysis half-life is 6.6 days at 70° C and pH 7.1 (6), but no activation energy was determined with which to extrapolate the hydrolysis rate to lower temperatures. The photolysis half-life of 1,2,4-trichlorobenzene in surface water at 40° latitude in summer, calculated from measured quantum yields and spectral data was 450 years (3). Product studies for photolysis in water gave no evidence for either dichlorophenols or dichlorobenzenes (3). However, another study found that the primary photohydrolysis products were dichlorophenols, but these were subject to secondary reactions (4).

1,2,4-Trichlorobenzene reacts with photochemically-produced hydroxyl radicals in the atmosphere with a rate constant of $5.32 \times 10^{-13} \text{ cm}^3/\text{molecule-s}$ (5). Assuming a hydroxyl radical concentration of $5 \times 10^5 \text{ radicals/cm}^3$, the half-life of 1,2,4-trichlorobenzene is 30.2 days. 1,2,4-Trichlorobenzene absorbs radiation >290 nm and therefore can undergo direct photolysis. However, since the overlap between the absorption spectrum and the solar spectrum is so small, the maximum rate of photolysis in the atmosphere for midday in mid-summer is only 0.03%/hour (7). Exposure of 20 grams 1,2,4-trichlorobenzene in borosilicate glass flask to sunlight for 56 days resulted in the formation of 9,770 ppm of at least six pentachlorobiphenyl isomers (2).

1,2,4-Trichlorobenzene biodegrades in laboratory tests using acclimated microorganisms (8, 9, 10, 11). Biodegradability proceeds rapidly when 1,2,4-trichlorobenzene is incubated with inocula that are acclimated to textile chemicals, rather than those from "typical treatment plants" (9). In one BOD test which used a seed from an industrial wastewater treatment plant that was not especially acclimated to 1,2,4-trichlorobenzene, 1,2,4-trichlorobenzene disappearance was noted after one day and 99% disappearance was obtained in ten days, although no oxygen uptake was noted until day 10 (9). The BOD

after 10 days was 55% (9). Five days after ^{14}C -1,2,4-trichlorobenzene was incubated with activated sludge from an industrial wastewater plant, 56% of the 1,2,4-trichlorobenzene was converted to CO_2 , 7% had volatilized, and 23% was converted to polar metabolites (9). Eighty percent of the unchanged 1,2,4-trichlorobenzene was adsorbed on solids. The influent of an advanced wastewater treatment plant contained 0.11 to 0.46 ppt of 1,2,4-trichlorobenzene while the effluent contained ND to 0.01 ppt (15).

1,2,4-Trichlorobenzene very slowly biodegraded in a sandy loam soil; the mineralization rate was 0.181 $\mu\text{g/day}$ in 20 g of soil (12). Little or no mineralization occurred when 1,2,4-trichlorobenzene was aerobically incubated with saturated subsurface soil (13). 1,2,4-Trichlorobenzene is reductively dechlorinated to monochlorobenzene via 1,4-dichlorobenzene in anaerobic sediment columns (14).

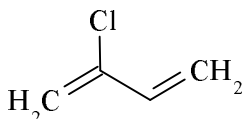
[(1) Schmidt-Bleek F et al; Chemosphere 11: 383-415 (1982) (2) Uyeta M et al; Nature 264: 583-4 (1976) (3) Dulin D et al; Environ Sci Technol 20: 72-7 (1986) (4) Boule P et al; Photochemistry of environmental aquatic systems pp. 10-26. ACS Symposium Series, Washington, DC: American Chemical Society (1987) (5) Atkinson R; Chem Rev 85: 69-201 (1985) (6) Ellington JJ et al; Measurement of hydrolysis rate constants for evaluation of hazardous waste land disposal Volume 1 EPA/600/3-86/043 pp. 82-84 (1987) (7) Bunce NJ et al; Environ Sci Technol 23: 213-218 (1989) (8) Tabak HH et al; J Water Pollut Control Fed 53: 1503-18 (1981) (9) Simmons P et al; Text Chem Color 9: 211-3 (1977) (10) Malaney GW, McKinney RE; Water Sew Works 113: 302-9 (1966) (11) Gaffney PE; J Water Pollut Control Fed 48: 2731-7 (1976) (12) Marinucci AC, Bartha R; Appl Environ Microbiol 38: 811-7 (1979) (13) Aelion CM et al; Appl Environ Microbiol 53: 2212-7 (1987) (14) Bosma TNP et al; FEMS Microbiol Ecol 53: 223-9 (1988) (15) Reinhard M, McCarty PL; Chem Water Reuse 2: 33-53 (1981)]

CHLOROPRENE

SUBSTANCE IDENTIFICATION

Synonyms: 2-Chloro-1,3-butadiene; β -chloroprene

Structure:



CAS Registry Number: 126-99-8

Molecular Formula: C_4H_5Cl

CHEMICAL AND PHYSICAL PROPERTIES

Boiling Point: 59.4 °C

Melting Point: -130 °C

Molecular Weight: 88.54

Dissociation Constants: Not applicable

Log Octanol/Water Partition Coefficient (log K_{ow}): 2.53 (estimated, 1)

Water Solubility: 250 mg/L (3)

Vapor Pressure: 174 mm Hg @ 20 °C (2)

Henry's Law Constant: 8.1×10^{-2} atm-m³/mole (calculated from the vapor pressure and water solubility)

Lower Explosive Limit: 4% @ 20 °C (4)

[(1) Meylan WM, Howard PH; Group contribution method for estimating octanol-water partition coefficients. SETAC Meeting Cincinnati, OH. Nov 8-12, (1992)] (2) Boublik T et al; The Vapor Pressures of Pure Substances Amsterdam: Elsevier (1984) (3) Kleinschmidt P; Ullmann's Encyclopedia of Industrial Chemistry A6: 315-318 1986) (4) NPFA; Fire Protection Guide to Hazardous Materials 9th Edition, p. 325M (1986)]

EXPOSURE PROFILE

Production: Production of chloroprene can be approximately equated to the amount of polychloroprene (neoprene) produced. Excluding Russia, China, and Eastern Bloc countries, polychloroprene production was 321,000 tons in 1989; approximately half of this was consumed in the United States (1). In the U.S., chloroprene is produced by Du Pont and Mobay (1).

[(1) Stewart CA Jr; Kirk-Othmer Encyclopedia of Chemical Technology, 4th ed. 6: 70-78 (1993)]

Use: Chloroprene is almost entirely used in the production of polychloroprene synthetic rubbers (1). The only other use having any significant volume is the manufacture of 2,3-dichloro-1,3-butadiene which is used as a monomer in copolymerizations with chloroprene (1).

[(1) Stewart CA Jr; Kirk-Othmer Encyclopedia of Chemical Technology, 4th ed. 6: 70-78 (1993)]

Occupational Exposure: NIOSH (NOES Survey 1981-83) has statistically estimated that 17,749 workers are exposed to chloroprene in the United States (1). In a survey of a neoprene production facility in 1979, chloroprene concentrations ranged up to 1200 ppm with 53% of the samples exceeding the NIOSH recommended standard of 1.0 ppm and 0.5% of the samples exceeded the OSHA standard of 25 ppm (2). In two other neoprene production facilities, chloroprene concentrations were 0.14-0.18 ppm and below the limits of detection, respectively (3, 4). Chloroprene levels of up to 0.2 ppm were reported in air in a metal fabricating plant where polychloroprene was applied to metal cylinders prior to vulcanization (5). Air levels of chloroprene in a polymerization plant ranged from 14 to 1420 ppm in the make-up area, from 130 to 6760 ppm in the reactor area, from 6 to 440 in the monomer recovery area, and from 113 to 252 ppm in the latex area (5).

[(1) NIOSH. National Institute for Occupational Safety and Health. National Occupational Exposure Survey (NOES). Computer printout March 29, 1989 (2) McGlothlin JD et al; Health Hazard Evaluation Report No. HETA-79-027-1459, E.I. DuPont De Nemours & Co., Louisville, Kentucky. Health Evaluation and Technical Assistance Branch, NIOSH, Cincinnati, Ohio (1984) (3) Anonymous; Walk-Through Survey Report, Nazar Rubber Company, Toledo, Ohio. NIOSH/00113364. Division of Surveillance, Hazard Evaluations and Field Studies, NIOSH, Cincinnati, Ohio (1977) (4) Wallingford KM; Bowman LL; Survey Report of Cincinnati Rubber Manufacturing Company, Norwood, Ohio, Report No. IWS-087-12. NIOSH/00194763. Industry-Wide Studies Branch, Division of Surveillance, Hazard Evaluations and Field Studies, NIOSH, Cincinnati, Ohio (1977) (5) IARC; 2-Chloro-1,3-butadiene and Polychloroprene 19: 131-5 (1979)]

Consumer Exposure: Since chloroprene is used only as an intermediate in polymer production, no consumer exposure is anticipated.

Environmental Release and General Population Exposure: According to the 1991 Toxics Release Inventory (TRI), 1,678,535 pounds of chloroprene were released to the environment, of which 87.6% was released into the atmosphere and 8.2% to land (1). Chloroprene was detected in the all six New Jersey cities sampled; the mean and maximum concentrations were 0.097 ppb and 4.0 ppb, respectively (2). In Houston, TX and Baton Rouge, LA, the respective air concentrations of chloroprene were 0.59 ppb and below the detection limit (3). Chloroprene was detected in only 1 out of 204 samples of surface water taken from sites near heavily industrialized areas across the U.S. during 1975-1976 (4). In a comprehensive survey of wastewater from 4,000 industries and publicly-owned treatment plants (POTWs) by EPA, chloroprene was identified in discharges from the following industrial categories (frequency of occurrence - number of plants; median concentration in ppb): organics and plastics (3; 1750); plastics and synthetics (1; 507); rubber processing (1; 494); and photographic industries (1; 4.8) (5).

[(1) U.S. EPA; Toxics Release Inventory (1992) (2) Harkov R et al; pp. 104-19 In: Proc Int Tech Conf Toxic Air Contam McGovern JJ ed. APCA. Pittsburgh, PA (1981) (3) Brodzinsky R, Singh HB; Volatile organic chemicals in the atmosphere: An assessment of available data. SRI International. Menlo Park CA (1982) (4) Ewing BB et al; Monitoring to

detect previously unrecognized pollutants in surface waters EPA 560/6-77-015 (1977) (5) Shackelford WM et al; *Analyt Chim Acta* 146:15-27 [supplementary data] (1983)]

Environmental Transport and Persistence:

Bioaccumulation: A biconcentration factor (BCF) of 49 is estimated for chloroprene from its log octanol/water partition coefficient using a recommended regression equation (1). This low BCF value suggests that chloroprene will not bioaccumulate significantly in aquatic organisms.

[(1) Lyman WJ et al; *Handbook of Chem Property Estimation Methods* Washington, DC: American Chemical Society p. 5-5 (Eqn 5-2) (1990)]

Volatilization/ Adsorption: According to a simple fugacity model, the mass distribution of chloroprene among the environmental compartments at equilibrium is 0.9994 in air, 0.0006 in water, and 0.0000 in soil (4). Using the estimated Henry's Law constant, the volatilization half-life for chloroprene from a model river 1 m deep with a current velocity of 1 m/sec and a wind speed of 3 m/sec is estimated to be 2.8 hours (1). Its volatilization half-life from a model lake 1 m deep with a 0.05 m/s current and 0.5 m/s wind is estimated to be 3.7 days (1). Based on a quantitative structure-activity analysis, a soil adsorption coefficient (K_{oc}) of 68 is estimated for chloroprene (2). This indicates that adsorption to suspended solids and sediments in water would not be significant and chloroprene would be mobile in soil (3). Chloroprene's high vapor pressure, low Henry's Law constant, and low adsorptivity to soil indicates that it would rapidly volatilize from wet and dry soil.

[(1) Lyman WJ et al; *Handbook of Chem Property Estimation Methods* Washington, DC: American Chemical Society pp. 15-12 to 15-34 (1990) (2) Meylan WM et al; *Environ Sci Technol* 26:1560-7 (1992) (3) Swann RL et al; *Res Rev* 85: 17-28 (1983) (4) U.S. EPA; PCGEMS (Graphical Exposure Modeling System), PCENPART (Environmental Partitioning Model)]

Persistence: Chloroprene is a highly reactive chemical to which inhibitors are added to prevent spontaneous polymerization in the presence of air. As an added precaution, it is stored and transported under inert gas at low temperatures (3). Therefore, chloroprene may be expected to react with oxygen and free radicals in the environment. Based on its vapor pressure, chloroprene is expected to exist almost entirely in the vapor phase in the atmosphere (1). In the atmosphere, it will react with photochemically-produced hydroxyl radicals with an estimated rate constant of 2.1×10^{-11} cm³/molecule-s (2) for abstraction of a hydrogen atom. Assuming a hydroxyl radical concentration of 5×10^5 radicals/cm³, the half-life of chloroprene is 18.3 hours. The reaction of chloroprene with atmospheric ozone is estimated to be 1.16×10^{-18} cm³/molecule-s (2). Assuming an ozone concentration of 7×10^{11} molecules/cm³, the half-life is 9.9 days. Therefore, the reaction with hydroxyl radicals will be the dominant degradation pathway for chloroprene in the atmosphere. No information concerning chloroprene's biodegradability was located.

[(1) Eisenreich SJ; Environ Sci Tech 15: 30-8 (1981) (2) Meylan WM, Howard PH; Chemosphere 26: 2293-2299 (1993) (3) Kleinschmidt P; Ullmann's Encyclopedia of Industrial Chemistry A6: 315-318 1986)]

CARBONYL SULFIDE

SUBSTANCE IDENTIFICATION

Synonyms: Carbon oxysulfide

Structure:



CAS Registry Number: 463-58-1

Molecular Formula: COS

CHEMICAL AND PHYSICAL PROPERTIES

Boiling Point: -50.2

Melting Point: -138.8

Molecular Weight: 60.07

Dissociation Constants: Not applicable

Log Octanol/Water Partition Coefficient (log K_{ow}): 0.800

Water Solubility: 1,220 mg/L (1)

Vapor Pressure: 9,410 mm Hg @ 25 °C (2)

Henry's Law Constant: 5.06×10^{-2} atm-m³/mole (3)

Lower Explosive Limit: 12% @ 25 °C (4)

[(1) Macaluso P; Kirk-Othmer Encyclopedia of Chemical Technology 2nd ed New York, NY: Wiley 19: 371-424 (1969)

(2) Daubert TE, Danner RP; Physical & Thermodynamic Properties of Pure Chemicals Volume 1 New York, NY:

Hemisphere Pub Corp (1989) (3) Yaws C et al; Chem Eng pp. 179-85 (November) (1991) (4) Parmeggiani L;

Encyclopedia of Occupational Health and Safety p. 2124 (1983)]

EXPOSURE PROFILE

Production: No non-CBI production volumes are available for carbonyl sulfide. According to the 1991 Toxics Release Inventory (TRI), 36 U.S. facilities produced carbonyl sulfide as an impurity or byproduct (1). Of these, 2 facilities (Sid Richardson Carbon and Gasoline Company in West Baton Rouge, LA, and Big Springs, TX) utilized carbonyl sulfide for on-site use/processing (1).

[(1) U.S. EPA; Toxics Release Inventory (1992)]

Use: The commercial importance of carbonyl sulfide is limited; it is not produced in large quantities and it is used only for small-scale synthesis and experiments (1). Previous uses of carbonyl sulfide were for the synthesis of thio organic compounds (2), including the synthesis of the herbicide triallate (3).

[(1) Lay DS et al; pp. 185-95 In: Ullmann's Encyclopedia of Industrial Chemistry New York, NY: VCH Publ (1986) (2) Hawley CG; The Condensed Chemical Dictionary 10th ed New York, NY: Van Nostrand Reinhold Co p. 198 (1981) (3) Leiber MA, Berk HC; Anal Chem 57: 2792-2796 (1985)]

Occupational Exposure: No data on occupational exposure to carbonyl sulfide could be located in the available literature. Carbonyl sulfide emissions are associated with coal-fired power plants, biomass combustion, fish processing, combustion of refuse and plastics, petroleum, synthetic fiber, starch, rubber, and paper manufacture, and shale oil retorting and coal conversion facilities (1-4). Workers in these, and related industries, may potentially be subject to carbonyl sulfide by inhalation. Occupational exposure to carbonyl sulfide may also occur due to its presence in automobile and diesel exhaust (1, 2).

[(1) Khalil MAK, Rasmussen RA; Atmos Environ 18: 1805-13 (1984) (2) Hanson RL et al; Arch Environ Contam Toxicol 14: 289-97 (1985) (3) DeSousa TLC; J Chromatog 395: 413-22 (1987) (4) Sklarew DS et al; Environ Sci Tech 18: 592-600 (1984)]

Consumer Exposure: No data are available to indicate that carbonyl sulfide is present in consumer products.

Environmental Release and General Population Exposure: According to the 1991 TRI, 16.7 million pounds (8,350 tons) of carbonyl sulfide were released to the environment, all of which was released into the atmosphere (1). Carbonyl sulfide may be released to the environment from automobile and diesel exhaust (2, 3), coal-fired power plants, biomass combustion, fish processing, combustion of refuse and plastics, petroleum, synthetic fiber, starch, rubber (2) and paper manufacture (4), and shale oil retorting and coal conversion facilities (3, 5). Annual industrial emissions of carbonyl sulfide in the Netherlands during 1980 amounted to 46 tons/year, all from stationary sources (6). The tropospheric burden of carbonyl sulfide is estimated as 4.4 million tons/year (7). Estimated average emissions of carbonyl sulfide from anthropogenic sources are 0.44 million tons/year (range 0.32-0.88 million tons/year) from biomass burning and 0.12 million tons/year (range 0.02-0.6 million tons/year) from automobiles, chemical industries, and sulfur recovery processes (2). Anthropogenic emissions of carbonyl sulfide have been estimated to be less than one third that of natural emissions (2). The average concentration of carbonyl sulfide in the waste gas from two different shale oil retorting facilities were 394 ppm and 13 ppm (5). It was detected in 1 out of 63 effluent samples obtained from a wide range of chemical manufacturing in areas across the U.S. (6).

Estimated emissions of carbonyl sulfide from natural sources total 5.8-7.68 million tons/year from oceanic emissions (0.88 million tons/year), salt marshes (0.26 million tons/year), inland swamps (4.0 million tons/year), soil and plants (0.44-2.2 million tons/year), biomass burning (0.24 million

tons/year), and volcanoes and fumaroles (0.022 million tons/year) (2). Emissions of carbonyl sulfide have also been associated with deciduous trees, coniferous trees, salt marshes, and soils (9). The mean carbonyl sulfide emissions were 17.3 µg/day from a hardwood forest and 39.7 µg/day from a pine forest; the emission rate increased dramatically after the addition of fertilizer (10). The average emission of carbonyl sulfide from 5 different soil types was found to range from 0.0028 to 7.8 g/m³-year (11). Carbonyl sulfide may be formed in the atmosphere by the gas-phase reaction of carbon disulfide and photochemically produced hydroxyl radicals (12).

The atmospheric concentrations of carbonyl sulfide reported in several studies published between 1975 and 1977 were 423-1253 ppt at various locations in the U.S., 391-2350 ppt in the U.K., 1833 ppt in Philadelphia, PA, 1896 ppt in Wallops Island, VA, and 2147 ppt in Lawton, OK (13). The concentration of carbonyl sulfide in Harwell, England, date not given, ranged from 400 to 560 ppt (14). Carbonyl sulfide was found in 1 of 8 personal air samples of subjects monitored in Bayonne and Elizabeth, NJ (15). The world-wide average atmospheric concentration of carbonyl sulfide is relatively constant at 500 ppt (10). The concentration of carbonyl sulfide measured during airplane flights over the remote Azores Islands and Bavaria, Germany, ranged from 450 to 550 ppt (16). The concentration of carbonyl sulfide in air ranged from 627 to 690 ppt at an altitude between 180 and 1950 m (17). Reported concentrations of carbonyl sulfide in water range from 60 to 180 ppt in salt marshes and 14 to 19 ppt in the ocean (18).

Members of the general population are exposed to carbonyl sulfide by inhalation due to its presence in air. Higher levels of exposure may occur by inhalation of automobile and diesel exhaust, or during operations which involve burning biomass. Carbonyl sulfide was qualitatively detected in 1 of 8 samples of mother's milk obtained from residents of urban centers in PA, NJ, and LA (19)

[(1) U.S. EPA; Toxics Release Inventory (1992) (2) Khalil MAK, Rasmussen RA; Atmos Environ 18: 1805-13 (1984) (3) Hanson RL et al; Arch Environ Contam Toxicol 14: 289-97 (1985) (4) DeSousa TLC; J Chromatog 395: 413-22 (1987) (5) Sklarew DS et al; Environ Sci Tech 18: 592-600 (1984) (6) Guichert R, Schulting FL; Sci Total Environ 43: 193-219 (1985) (7) Sze ND, Ko MK; Atmos Environ 14: 1223-29 (1980) (8) Perry DL et al; Identification of organic compounds in industrial effluent discharges EPA-600/4-79-016, NTIS PB-294794 (1979) (9) Aneja VP; J Air Waste Manag Assoc 40: 469-76 (1990) (10) Melillo JM, Steudler PA; J Atmos Chem 9: 411-7 (1989) (11) Adams DF et al; J Air Pollut Contr Fed 29: 380-3 (1979) (12) Sze ND, Ko MKW; Nature 280: 308-10 (1979) (13) Aneja VP et al; J Air Pollut Contr Fed 32: 803-7 (1982) (14) Sandalls FJ, Penkett SA; Atmos Environ 11: 197-9 (1977) (15) Wallace LA et al; Environ Res 35: 293-319 (1984) (16) Ockelmann G et al; Comm Eur Communities Atmos Pollut: 596-603 (1987) (17) Mihalopoulos N et al; Atmos Environ 23: 2159-66 (1989) (18) Kelly DP, Smith NA; Adv Microb Biol 11: 345-85 (1990) (19) Pellizzari ED et al; Bull Environ Contam Toxicol 28: 322-8 (1982)]

Environmental Transport and Persistence:

Bioaccumulation: Estimated bioconcentration factors ranging from 2 to 11 based on its water solubility and log octanol/water partition coefficient (1) indicate that carbonyl sulfide will not bioconcentrate in fish or aquatic organisms.

[(1) Lyman WJ et al; Handbook of Chemical Property Estimation Methods. Environmental Behavior of Organic Compounds. New York, NY: McGraw-Hill pp. 5.1-5.30 (1982)]

Volatilization/ Adsorption: According to a simple fugacity model, the mass distribution of carbonyl sulfide among the environmental compartments at equilibrium is 0.04% to water, 99.96% to air, and none to soil (1). The half-life for volatilization of carbonyl sulfide from a model river and lake are approximately 1 hour and 3 days, respectively (2). Estimated soil adsorption coefficients ranging from 65 to 88 based on its water solubility and log octanol/water partition coefficient (2) indicate that carbonyl sulfide will display high mobility (3). Volatilization of carbonyl sulfide from both dry and moist soil is expected to be rapid in light of its high vapor pressure, high Henry's Law constant, and limited potential for adsorption to soil.

[(1) U.S. EPA; PCGEMS (Graphical Exposure Modeling System), PCENPART (Environmental Partitioning Model) (2) Lyman WJ et al; Handbook of Chemical Property Estimation Methods. Environmental Behavior of Organic Compounds. New York, NY: McGraw-Hill pp. 4.1-4.33 (1982) (3) Swann RL et al; Res Rev 85: 17-28 (1983)]

Persistence: Carbonyl sulfide is expected to have a long residence time in the atmosphere with estimates ranging from 200 to 7300 days (1). The atmospheric life-time of carbonyl sulfide, based on removal via the gas-phase reaction with photochemically produced hydroxyl radicals and oxygen, direct photolysis, and unknown removal processes invoked to balance the sulfur cycle is approximately 2 years (2). Studies have shown that carbonyl sulfide may be adsorbed from the atmosphere by plants and by moist soil, the latter due to microbial uptake (3, 4). Experimental rate constants for the gas-phase reaction of carbonyl sulfide with photochemically produced hydroxyl radicals ranging from 6.08×10^{-12} to $8.8 \times 10^{-15} \text{ cm}^3/\text{molecule-sec}$ have been measured (5-7) and translate to atmospheric half-lives ranging from 500 days to 6.5 years. Carbonyl sulfide is not expected to undergo direct photolysis in the troposphere, but it may in the stratosphere (8).

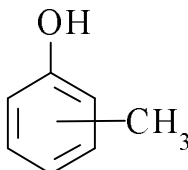
[(1) Aneja VP et al; J Air Pollut Contr Fed 32: 803-7 (1982) (2) Khalil MAK, Rasmussen RA; Atmos Environ 18: 1805-13 (1984) (3) Mihalopoulos N et al; Atmos Environ 23: 2159-66 (1989) (4) Bremner JM, Banwart WL; Biol Biochem 8: 79-83 (1976) (5) Kurylo MJ; J Photochem 9: 124-6 (1978) (6) Atkinson R et al; Chem Phys Lett 54: 14-18 (1978) (7) Cox RA, Sheppard D; Nature 284: 330-1 (1980) (8) Baulch DL et al; J Phys Chem Ref Data 13: 1259-1380 (1984)]

CRESOL

SUBSTANCE IDENTIFICATION

Synonyms: Methylphenol; cresylic acid; cresylol; tricresol; hydroxytoluene

Structure:



CAS Registry Numbers: 1319-77-3 (mixture of 3 isomers)
95-48-7 (*ortho*- isomer)
108-39-4 (*meta*- isomer)
106-44-5 (*para*- isomer)

Molecular Formula: C₇H₈O

CHEMICAL AND PHYSICAL PROPERTIES

Boiling Points: 191-192°C (*ortho*-)
202°C (*meta*-)
201.8°C (*para*-)

Melting Points: 30°C (*ortho*-)
11-12°C (*meta*-)
35.5°C (*para*-)

Molecular Weight: 108.13

Dissociation Constants: 10.287 (*ortho*-) (1)
10.09 (*meta*-) (1)
10.26 (*para*-) (1)

Log Octanol/Water Partition Coefficients (log K_{ow}): 1.95 (*ortho*-) (2)
1.96 (*meta*-) (2)
1.94 (*para*-) (2)

Water Solubilities: 25,950 mg/L @ 25°C (*ortho*-) (3)
22,700 mg/L @ 25°C (*meta*-) (3)
21,520 mg/L @ 25°C (*para*-) (3)

Vapor Pressures: 0.26 mm Hg @ 25°C (*ortho*-) (4)
0.14 mm Hg @ 25°C (*meta*-) (4)
0.083 mm Hg @ 25°C (*para*-) (4)

Henry's Law Constants: 1.2 x 10⁻⁶ atm-m³/mole @ 25°C (*ortho*-) (5)
8.6 x 10⁻⁷ atm-m³/mole @ 25°C (*meta*-) (estimated from

the vapor pressure and the water solubility, 6)
1.0 x 10⁻⁶ atm-m³/mole @ 25 °C (*para*-) (5)
≤ 1.35% @ 300 °F (mixture of 3 isomers) (6)

Lower Explosive Limit:

[(1) Riddick JA et al; Organic Solvents New York: Wiley Interscience pp. 244-249 (1986) (2) Hansch C, Leo AJ; Medchem Project Issue No 26 Claremont, CA: Pomona College (1985) (3) Yalkowsky SH; The Fifth edition of the Aquasol database of aqueous solubility. College of Pharmacy, University of Arizona, Tucson, AZ (1992) (4) Chao J et al; J Phys Chem Ref Data 12: 1033-63 (1983) (5) Gaffney JS et al; Environ Sci Technol 21: 519-23 (1987) (6) Lyman WJ et al; Handbook of Chemical Property Estimation Methods, Washington, DC: American Chemical Society Chapter 15 (1990) (6) Sax NI; Dangerous Properties of Industrial Materials 6th Edition, p. 814 (1984)]

EXPOSURE PROFILE

Production: No data were located regarding current non-CBI production volumes of individual cresol isomers or specific cresol mixtures. In 1990, the U.S. production of cresols and cresylic acid, excluding data from coke oven and gas-retort ovens, was 84.3 million pounds (1). The commercial mixture of cresol isomers, in which the *meta*- isomer predominates, is sometimes referred to as cresylic acid (2) or cresylics (4). Cresylic acids contain cresols and small amounts of phenols and xylenols and they are defined as those mixtures in which over 50% will boil above 204 °C (3). In 1990, the national capacity for producing cresylics was 206 million pounds per year (4). *ortho*-Cresol is produced by Aldrich Chemical Co. (Milwaukee, WI), General Electric Co. (Selkirk, NY), Merichem Co. (Houston, TX), and PMC, Inc. (Chicago, IL) (5). *meta*-Cresol is produced by Aldrich Chemical Co. (Milwaukee, WI), Merichem Co. (Houston, TX), and Rhone-Poulenc Inc (Oil City, PA) (5). *para*-Cresol is produced by Aldrich Chemical Co. (Milwaukee, WI), Bell Flavors & Fragrances Inc. (Northbrook, IL and Oakland, NJ), Merichem Co. (Houston, TX), and PMC, Inc. (Chicago, IL) (5).

[(1) USITC; Synthetic Organic Chemicals. United States Production and Sales, 1990. USITC Publication 2470. pp. 3-2, 3-5. December (1991) (2) Budavari S et al; The Merck Index. 11th ed Merck & Co., Inc. Rahway, NJ. p. 404 (1989) (3) Hawley's Condensed Chemical Dictionary. 11th ed New York, NY: Van Nostrand Reinhold p. 320-2 (1987) (4) Chemical Marketing Reporter; Chemical Profile: Cresylics October 22 (1990) (5) SRI International; 1993 Directory of Chemical Producers, United States of America pp. 533-4 (1993)]

Use: *ortho*-Cresol is primarily used as either a solvent or disinfectant. It is also used as a chemical intermediate for a wide variety of products including 2-methylcyclohexanol, 2-methylcyclohexanone, coumarin, and 3-isopropyl-6-methylphenol (carvacrol) (1, 2). *ortho*-Cresol is also used in the manufacture of several antioxidants, dyes, and in the formation of epoxy-*o*-cresol novolak (ECN) resins (3). ECN resins are sealing materials for integrated circuits (silicon chips) (3). *ortho*-Cresol is also used as an additive to phenol-formaldehyde resins (3). Furthermore, the manufacture of certain herbicides and pesticides, including 4-chloro-2-methylphenoxyacetic acid (MCPA), 2-(4-chloro-2-methylphenoxy)-propionic acid (MCP), γ -(4-chloro-2-methylphenoxy)-butyric acid (MCPB), and 4,6-dinitro-*o*-cresol (DNCO), is dependent upon *ortho*-cresol (3).

meta-Cresol, either pure or mixed with *para*-cresol, is important in the production of contact herbicides such as O,O-dimethyl-O-(3-methyl-4-nitrophenyl)thionophosphoric acid (fenitrothion) and O,O-dimethyl-O-(3-methyl-4-methylthiophenyl)thionophosphoric acid ester (fenthion) (3). *meta*-Cresol is also used as a precursor to pyrethroid insecticides (3). Many flavor and fragrance compounds, such as (-)-methanol and musk amberette, are derived from *meta*-cresol. Furthermore, *meta*-cresol is used in the manufacture of the explosive, 2,4,6-trinitro-*m*-cresol (3).

para-Cresol is largely used in the production of antioxidants such as 2,6-di-*tert*-butyl-*p*-cresol (BHT), 2,6-dicyclopentyl-*p*-cresol, 2,2'-methylene- or 2,2'-thiodiphenols, and Tinuvin 326 (3). Tinuvin 326 is a substituted hydroxyphenyl benzotriazole (2) which is an absorber of UV light and is used in films and coatings (3). *para*-Cresol also has many applications in the fragrance and dye industries (1). *para*-Cresol carboxylic acid esters and anisaldehyde are used in perfumes (2).

Mixtures of *meta*- and *para*-cresol often serve as disinfectants and preservatives (1). Cresols are added to soaps and disinfectants. They are used as wood preservatives, in ore flotation, and in fiber treatment. *meta*- and *para*-Cresol mixtures are used in the manufacture of tricresyl phosphate and diphenyl cresyl phosphate, which are used in flame-retardant plasticizers for polyvinylchloride (PVC) and other plastics, fire-resistant hydraulic fluids, additives for lubricants, and air filters. Cresols are used in paints, textiles, modifying phenolic resins, as solvents for synthetic resin coatings such as wire enamels, metal degreasers, and cutting oils, and as agents to remove carbon deposits from combustion engines (1, 2, 3).

Cresylics are used in antioxidants (20%), phenolic-epoxy and novolak resins (15%), wire enamel solvents (12%), phosphate esters (5%), as chemical intermediates (5%), and in miscellaneous applications (8%), which include cleaning and disinfectant compounds and ore flotation (4).

[(1) Budavari S et al; The Merck Index. 11th ed Rahway, NJ: Merck & Co., Inc. p. 404 (1989) (2) Hawley's Condensed Chemical Dictionary. 11th ed New York, NY: Van Nostrand Reinhold. pp. 320-322, 1157 (1987) (3) Fiege H; Cresols and Xylenols Ullmann's Encyclopedia of Industrial Chemistry Volume A8: 25-59 (1987) (4) Chemical Marketing Reporter; Chemical Profile: Cresylics October 22 (1990)]

Occupational Exposure: NIOSH (NOES Survey 1981-83) has statistically estimated that 132,742 workers are potentially exposed to cresol (CAS Registry number 1319-77-3) in the U.S.; 10,985, 5,615, and 21,313 workers are potentially exposed to the *ortho*-, *meta*-, and *para*-isomers, respectively, in the United States (1). Occupational exposure to cresol may occur via inhalation of contaminated air or through dermal contact. Occupational exposure has been reported in laboratories and coal gasification facilities (2), during application of insulation lacquers to copper wires (4, 8), in wood-preserving facilities (4), and during paint and varnish application (3, 7). Workers were exposed to less than 0.1 mg/m³ cresol during creosote impregnation of wood (5). In 1981 and 1982, workers of a bench scale coal conversion process were exposed to atmospheric concentrations of cresol less than 0.1 ppm (6). One study suggests that workers may be exposed to 0.5-5 mg/m³ cresol in emissions from welding or straightening painted steel,

depending upon the primer or paint used (7). During the application of insulation to copper and aluminum wires, workers were exposed to 0.4 to 2.2 mg/m³ cresol in their personal breathing zones (8).

[(1) NIOSH. National Institute for Occupational Safety and Health. National Occupational Exposure Survey (NOES). In: RTECS. Registry of Toxic Effects of Chemical Substances. Version May (1993) (2) Needham LL et al; Anal Lett 17: 1555-1565 (1984) (3) Angerer J, Wulf H; Int Arch Occup Environ Health 56: 307-21 (1985) (4) Nieminen E, Heikkila P; J Chromatogr 360: 271-8 (1986) (5) Heikkila PR et al; Scand J Work Environ Health 13: 431-7 (1987) (6) Dreibelbis WG et al; In: Cooke M, Dennis AJ, Ed. Polynuclear Aromatic Hydrocarbons: Mechanisms, methods and metabolism. Columbus, OH: Battell Press, pp.351-361 (1985) (7) Henriks-Eckerman ML et al; Am Ind Hyg Assoc J 51: 241-4 (1990) (8) Moseley CL, Handke JL; Health Hazard Evaluation Report (HETA-83-116-1570) Essex Group, Inc. Vincennes, IN. US Dept. of Health and Human Services (1985)]

Consumer Exposure: Cresol use in perfumes, antiseptics, disinfectants, pharmaceuticals, paint and varnish, and soaps (1-3) may result in consumer exposure to cresol via dermal contact or inhalation of vapor. However, no qualitative or quantitative consumer exposure data are available.

[(1) Fiege H; Cresols and Xylenols Ullmann's Encyclopedia of Industrial Chemistry Volume A8: 25-56 (1987) (2) Angerer J, Wulf H; Int Arch Occup Environ Health 56: 307-21 (1985) (3) Hawley's Condensed Chemical Dictionary. 11th ed New York, NY: Van Nostrand Reinhold pp. 320-322 and 1157 (1987)]

Environmental Release and General Population Exposure: Cresol is a natural coal tar and petroleum product and it is widely distributed in the environment. It is a metabolite of various microorganisms and it is found naturally in the urine of mammals; in one day, a human eliminates an average of 87 mg of *para*-cresol in the urine (3). Cresol is naturally contained in the extracts and water vapor distillates of several plants, including jasmine flower oil, cassia flower oil, easter lily oil, ylang ylang oil, in the floral oil of *Yucca gloriosa*, in peppermint, eucalyptus, and camphor oil, and in the essential oils of several plants of the genus *Artemisia*, of conifers, oak wood, and sandalwood (3).

According to the 1991 Toxics Release Inventory (TRI), 1.50 million pounds of cresol were released to the environment, of which 49.5% was released into the atmosphere (1). Most of the rest was injected underground (1).

Exposure of the general population to cresol may occur via inhalation of contaminated air; however, cresol has a short ambient life-time. Cresol is formed in the atmosphere as a result of the reaction of toluene with photochemically-produced hydroxyl radicals (8). Cresol is released to the ambient air either naturally or artificially in emissions from paint, turbines, automobile exhaust, forest fires, coal combustion, diesel fuel, glass fiber and starch manufacturing, tap water odor, animal waste, vegetation, wood pulping, wood and tobacco smoke (2), and municipal solid waste combustion (4). Vehicular traffic provides a constant source of cresol exposure to the general population and residents near coal- and petroleum-fueled facilities and municipal solid waste incinerators may be exposed to cresol in air. People living in homes or areas where homes are heated with coal, oil, or wood may also be exposed to cresol in air. Exposure of the general

population to cresol may also occur via inhalation of cigarette smoke. An individual who smokes two packs of cigarettes a day may inhale 0.56-3.28 mg-cresol/day (7).

The general population will be exposed to cresol via consumption of contaminated food. Cresol has been detected in tomatoes and tomato ketchup, cooked asparagus, various cheeses, butter, and oil (3). Beverages such as red wine, whiskey, distilled spirits (6), raw and roasted coffee, and black tea contain cresol (3). Fried, smoked, and barbecued foods may also contain cresol (3, 5).

There are several pathways by which cresol may be released to soil and water and it is important to keep in mind that, in general, cresols will rapidly degrade in most surface water and soil environments. First, cresol from human urine (3) may be released to surface waters; however, most cresol from this source is probably biodegraded at municipal sewage treatment facilities prior to release to surface waters. Rural and suburban septic tanks may release cresol to soil. Cresol is constantly released to land and water from several natural sources via excrement, microbial activity, and vegetation. Surface runoff from terrestrial sources (3) and release from wet deposition (9) will contribute cresol to soil and surface water. Cresol may be released to groundwater from hazardous waste sites and landfills. Cresol is present in emissions from tap water (2). Therefore, humans may be exposed to cresol via ingestion of drinking water. Surface waters used for recreation and transportation may be contaminated with cresol from motor vehicle exhaust (10, 11). Waste water effluents from coal gasification (12, 13) and liquefaction facilities (14), shale oil production sites (15,16), refineries (17, 18), and poultry processing plants (19) will release cresol to surface waters at concentrations ranging from about 0.001 to 1,840 mg/L. Subsequently, the general population may be exposed to cresol via dermal contact in surface waters during certain activities such as swimming. However, high levels of cresol in soil and water, constituting concern for exposure to the general population, would predominantly be released from accidental spills and fugitive discharges during the use, manufacture, transport, and storage of cresol or cresol products from the coal tar and petroleum industries.

[(1) U.S. EPA; Toxics Release Inventory (1992) (2) Graedel TE et al; Atmospheric Chemical Compounds Academic Press, Inc. Orlando, FL pp. 249-50 (1986) (3) Fiege H; Cresols and Xylenols Ullmann's Encyclopedia of Industrial Chemistry Volume A8: 25-56 (1987) (4) James H et al; J Proc - APCA 77th annual meeting June 24-9 San Francisco, CA paper 84-18.5 pp. 1-25 (1984) (5) Ho CT et al; J Agric Food Chem 31: 336-42 (1983) (6) Lehtonen M; J Assoc Off Anal Chem 66: 62-70 (1983) (7) Wynder EL, Hoffman D; Tobacco and Tobacco Smoke. New York, NY: Academic Press p. 387 (1967) (8) Leone JA et al; Int J Chem Kinet 17: 177-216 (1985) (9) Leuenberger C et al; Environ Sci Technol 19: 1053-58 (1985) (10) Hampton CV et al; Environ Sci Technol 16: 287-98 (1982) (11) Johnson LD et al; J Air Pollut Control Assoc 39: 709-13 (1989) (12) Giabbi MF et al; J Environ Anal Chem 20: 113-29 (1985) (13) Neufeld RD et al; J Water Pollut Control Fed 57: 955-64 (1985) (14) Fedorak PM, Hrudey SE; Water Res J 20: 929-33 (1986) (15) Dobson KR et al; Water Res 19: 849-56 (1985) (16) Hawthorne SB, Sievers RE; Environ Sci Technol 18: 483-90 (1984) (17) Cardwell TJ et al; Environ Anal Chem 24: 23-35 (1986) (18) Snider EH, Manning FS; Environ Int 7: 237-258 (1982) (19) Andelman JB et al; Water Res 18: 843-54 (1984)]

Environmental Transport and Persistence:

Bioaccumulation: Based on measured BCF values of 10.7 for *ortho*-cresol (1) and 20 for *meta*-cresol (2), bioconcentration in fish will not be important.

[(1) Sabljic A; Z Gesamte Hyg Ihre Grenzgeb 33: 493-6 (1987) (2) Frietag D et al; Chemosphere 14: 1589-616 (1985)]

Volatilization/ Adsorption: According to a simple fugacity model, cresol will distribute approximately 92% to water and 8% to air (5). Based on a suggested classification scheme (1) and an average Henry's Law constant of about 1×10^6 atm-m³/mole at 25°C for all three cresol isomers, cresol will volatilize slowly from most aquatic environments; however, under extreme conditions, volatilization may be important in shallow rapidly moving bodies of water. Based on the average Henry's Law constant, volatilization half-lives of 38.2 and 281 days can be estimated for a model river (1 m deep with a current velocity of 1 m/sec) and a model lake (1 m deep with a current velocity of 0.05 m/sec), respectively (1). Experimental K_{oc} values of 21.9, 34.6, and 48.7 for *ortho*-, *meta*-, and *para*-cresol (2), respectively, suggest that cresol has very high mobility in soil (3) and low adsorption potential. However, K_{oc} values from 115 to 3,420 were also experimentally determined for *para*-cresol (4). A K_{oc} value of 3,420 indicates slight mobility in soil (3) and a high adsorption potential. These inconsistencies are adequately described by hydrogen bonding between the phenolic hydroxyl group and active sites in the soil (4). Therefore, cresol may adsorb to soil depending upon the amount of hydrogen bonding taking place, which will depend upon the pH of the soil, the type of soil, the anion exchange capacity, and the amount of organic matter present.

[(1) Lyman WJ et al; Handbook of Chemical Property Estimation Methods. Environmental Behavior of Organic Compounds. Washington DC: American Chemical Society pp. 15-15 to 15-32 (1990) (2) Boyd SA; Soil Science 134: 337-43 (1982) (3) Swann RL et al; Res Rev 85: 17-28 (1983) (4) Southworth GR, Keller JL; Water Air Soil Pollut 28: 239-47 (1986) (5) U.S. EPA; PCGEMS (Graphical Exposure Modeling System), PCENPART (Environmental Partitioning Model)]

Persistence: The experimental rate constants for the reaction of *ortho*-, *meta*-, and *para*-cresol with photochemically-produced hydroxyl radicals are 4.2×10^{-11} , 6.4×10^{-11} , and 4.7×10^{-11} cm³/molecule-s, respectively (1). Assuming a hydroxyl radical concentration of 5×10^5 OH-radicals/cm³, the half-life for cresol will be 6-9.2 hours in the ambient atmosphere during the daytime. The rate of reaction with nitrate radicals is even higher (0.7×10^{-11} to 1.08×10^{-11} cm³/molecule-s (2, 3)) yielding a night-time half-life range of 4.5 to 6.9 minutes for cresol. Cresol was found to rapidly biodegrade in aerobic screening and sewage treatment plant simulation studies with half-lives of less than 24 hours to less than 7 days (4-18). Cresol isomers degraded in natural water grab samples under aerobic conditions with half-lives of less than 1 hour to 43 hours (19-22). Biodegradation in soil is also expected to be fast under aerobic conditions with half-lives of less than 0.6 days to 1.6 days (23-25). Under anaerobic conditions, however, biodegradation should be on the order of weeks to months (26-29)

[(1) Atkinson R; J Phys Chem Ref Data p. 233 (1989) (2) Atkinson R et al; Int J Chem Kinet 16: 887-98 (1984) (3) Carter WPL et al; Environ Sci Technol 15: 829-31 (1981) (4) Alexander M, Lustigman BK; J Agric Food Chem 14: 410-413 (1966) (5) Babeu L, Vaishnav DD; J Ind Microb 2: 107-115 (1987) (6) Baird RB et al; Arch Environ Contam Toxicol 2: 165-178 (1974) (7) Chambers CW et al; J Water Pollut Contr Fed 35: 1517-1528 (1963) (8) Heukelekian H, Rand MC; J Water Pollut Contr Assoc 29: 1040-1053 (1955) (9) Ludzack FJ, Ettinger

MB; J Water Pollut Control Fed 32: 1173-2000 (1960) (10) Lund FA, Rodriguez DS; J Gen Appl Microbiol 30: 53-61 (1984) (11) Malaney GW; J Water Pollut Control Fed 32: 1300-1311 (1960) (12) Malaney GW, McKinney RE; Water Sewage Works 113: 302-309 (1966) (13) McKinney RE et al; Sew Indust Wastes 28: 547-557 (1956) (14) Pauli O, Franke G; In: Proceedings of the 2nd International Biodeter Symposium. Biodeter Mater, 52-60 (1971) (15) Pitter P; Water Res 10: 231-235 (1976) (16) Singer PC et al; Treatability and assessment of coal conversion wastewaters. Phase I. Industrial Environmental Research Laboratory, U.S. EPA, Research Triangle Park, NC (1979) (17) Tabak HH et al; J Bacteriol 87: 910-919 (1964) (18) Young RHF et al; J Water Pollut Contr Fed R354 (1968) (19) Paris DF et al; Appl Environ Microbiol 45: 1153-1155 (1983) (20) Rogers JE et al; Battelle Pacific Northwest Labs, Richland, WA, 105. NTIS PB84-162866. EPA 600/3-84-043 (1984) (21) Smith JH et al; Environmental pathways of selected chemicals in freshwater systems. Part II: Laboratory studies. Environmental Research Laboratory, U.S. EPA, Research Triangle Park, NC pp. 6-27 (1978) (22) van Veld PA, Spain JC; Chemosphere 12: 1291-1305 (1983) (23) Namkoong W et al; Hazard Waste Hazard Mater 5: 321-328 (1988) (24) Medvedev VA, Davidov VD; In: Overcash MR, ed. Decomposition of toxic and nontoxic organic compounds in soil. Ann Arbor, MI: Ann Arbor Sci Publ., 175-181 (1981) (25) Medvedev VA, Davidov VD; In: Overcash MR, ed. Decomposition of toxic and nontoxic organic compounds in soil. Ann Arbor, MI: Ann Arbor Sci Publ., 245-254 (1981b) (26) Boyd SA et al; Appl Environ Microbiol 46: 50-54 (1983) (27) Fedorak PM, Hrudey SE; Water Res 18: 361-367 (1984) (28) Fedorak PM, Hrudey SE; Water Res 20(7): 929-933 (1986) (29) Fedorak PM et al; Water Res 20(10): 1315-1320 (1986)]

HYDROCHLORIC ACID

SUBSTANCE IDENTIFICATION

Synonyms: Hydrogen chloride; HCl

Structure:



CAS Registry Number: 7647-01-0

Molecular Formula: HCl

CHEMICAL AND PHYSICAL PROPERTIES

Boiling Point: -85.0 °C

Melting Point: -114.4 °C

Molecular Weight: 36.46

Dissociation Constants: $\text{pK}_a = -6.1$ (1)

Log Octanol/Water Partition Coefficient: Not available

Water Solubility: 41.2 mg/L @ 25 °C (3)

Vapor Pressure: 3.54×10^4 mm Hg @ 25 °C (2)

Henry's Law Constant: 2×10^6 atm-m³/mole @ 25 °C; under highly acidic conditions (4)

Lower Explosive Limit: Not available

[(1) Dean JA; Langes Handbook of Chemistry 13th ed McGraw-Hill Book Co. p. 5-15 (1985) (2) Daubert TE, Danner RP; Physical and Thermodynamic Properties of Pure Chemicals: Data Compilation Hemisphere Pub Corp New York, NY (1989) (3) Stephen H, Stephen T; Solubilities of inorganic and organic compounds In: Binary Systems. Stephen H et al. Eds, New York, NY p. 48 (1963) (4) Betterton EA; Gas Pollut: Character Cycl; Nriagu JO Ed, John Wiley & Sons, Inc. pp. 1-50 (1992)]

EXPOSURE PROFILE

Hydrochloric acid and hydrogen chloride are handled separately in industry. Hydrochloric acid is a solution of hydrogen chloride gas in water. In this document, HCl is used when addressing either chemical.

Production: In 1992, 5.75 billion pounds of HCl were produced in the United States (1). The manufacture of vinyl chloride from 1,2-dichloroethane is the major production source of HCl (1). U.S. producers of HCl are tabulated in Appendix A.

[(1) Reisch MS; Chemical and Engineering News pp. 10-13,16 April 12 (1993) (2) Austin S, Glowacki A; Hydrochloric acid In: Ullmann's Encyclopedia of Industrial Chemistry A13: 283-96 (1989)]

Use: HCl is the most important basic industrial chemical and the largest proportion of it is used immediately by the producer (1). HCl has many uses which include the manufacture of pharmaceutical hydrochlorides, vinyl chloride from acetylene, alkyl chlorides from olefins, and arsenious chloride from arsenious oxide (2). HCl is also used in the dissolution of minerals, pickling and etching of metals, regeneration of ion-exchange resins for water treatment, neutralization of alkaline products or waste materials, acidification of brine in chlor-alkali electrolysis, production of tin and tantalum, as an analytical reagent, deliming agent for hides, coagulation of latex, pH control, desulfurization agent for petroleum, hydrolyzing starch and proteins in the preparation of various food products, cleaning boilers, and heat-exchange equipment, pharmaceutical aid as acidifier, as a gastric acidifier in veterinary medicine, in the chlorination of rubber, as a gaseous flux for babbitting operations, and in isomerization, polymerization, and alkylation reactions (1-3). Other uses of HCl include phosphoric acid production, silica gel production, preparation of dyes and dye intermediates, reclamation of rubber, production of casein plastics, manufacture of paint pigments, and for etching airport runways in preparation for resurfacing with bonded concrete (4).

[(1) Austin S, Glowacki A; Hydrochloric acid In: Ullmann's Encyclopedia of Industrial Chemistry A13: 283-96 (1989) (2) Budavari S et al; The Merck Index. 11th ed Rahway, NJ: Merck & Co., Inc. pp. 756 and 759-60 (1989) (3) Curlin LC, Bommaraju TV; Kirk-Othmer Encyclopedia of Chemical Technology 4th ed New York, NY: John Wiley & Sons 1: 1000 (1991) (4) Kleckner WR, Sutter RC; Kirk-Othmer Encyclopedia Chemical Technology 2nd ed New York, NY: John Wiley & Sons 11: 333-4 (1966)]

Occupational Exposure: NIOSH (NOES Survey 1981-83) has statistically estimated that 1,131,879 workers are exposed to hydrochloric acid in the United States (1). During its use as an analytical reagent, workers in laboratories may be exposed to HCl. Workers in the finishing room of a polytetrafluoroethylene (PTFE) plant were exposed to up to 35 ppm HCl in the atmosphere immediately outside the oven where PTFE is heated above normal drying temperatures (2). HCl was qualitatively identified in the atmosphere of a nuclear submarine (3). In the chlorine production work area of a Texas chemical company, HCl was 1 of 3 chemicals that workers were principally exposed to (4). Workers employed in the meat packing department at Ashland Super Valu in Ashland, Wisconsin were exposed to 0.11 ppm HCl (5). Workers were exposed to less than 0.5-10 ppm HCl during normal welding operations of plasticized polyvinyl-chloride sheeting (6). Finnish workers were exposed to 0.5 ppm HCl in the air of the hot pressing area at a plant manufacturing particle board (7). HCl's use in etching (8) suggests that artists and craftsman may be exposed to it.

[(1) NIOSH. National Institute for Occupational Safety and Health. National Occupational Exposure Survey (NOES). Computer printout March 29 (1989) (2) Adams WGF; Trans Am Industr Med Offrs 13: 20-1 (1963) (3) Schaefer KE; Atmospheric Requirements of Confined Spaces 9: 320-31 (1964) (4) Bond GG et al; Am J Indust Med 7: 123-39 (1985) (5) Daniels WJ et al; Health Hazard Evaluation Report No. HETA-84-239-1586, Ashland Super Valu, Ashland, Wisconsin NIOSH U.S. Dept of Health and Human Services (1985) (6) Williamson J and Kavanagh B; Am Indust Hyg Assoc J 48: 432-6 (1987) (7) Kauppinen TP, Niemela RI; Scand J Work Environ Health 11: 357-63 (1985) (8) Austin S, Glowacki A; Hydrochloric acid In: Ullmann's Encyclopedia of Industrial Chemistry A13: 283-96 (1989)]

Consumer Exposure During its use in pH control and swimming pool treatment (1), people who use or maintain swimming pools may be exposed to HCl.

[(1) Chemyclopedia93; Kunej JH, Ed. American Chemical Society 11: 181-2 (1992)]

Environmental Release and General Population Exposure: According to the 1991 Toxics Release Inventory (TRI), 287.7 million pounds of hydrochloric acid were released to the environment, of which 28.8% was released into the atmosphere and 4.2% on land (1). Most of the rest was injected underground (1).

HCl may be released to the atmosphere as emissions from brick, ceramics, electronics, fertilizer, HCl, lacquer, polymer, and titanium manufacturing (2). It may also be released as emissions from forest fires, volcanoes, sewage treatment, sea salt, rockets, coal combustion, and automobiles (1). Up to 98% of the chlorine in coal is emitted as HCl from a coal-fired power plant (4). Air concentrations of HCl were 3 mg/m³ in emissions from a modern German municipal waste incinerator (5). HCl is also released in emissions from biomedical waste incinerators (6).

Based on the above data, residents downwind from effluent stacks may be exposed to HCl in air and people living in homes or areas where homes are heated with coal may be exposed to HCl in air. During the uses of HCl as a lab reagent and in etching (3), students in high school and college laboratories and artrooms may be exposed to HCl.

Small concentrations of free HCl occur naturally in the environment (3). HCl has been detected in the stratosphere at levels of ca. 1×10^{-11} vol% and the concentration of HCl in the human stomach is about 0.1 mol/L (3).

[(1) U.S. EPA; Toxics Release Inventory (1992) (2) Graedel TE et al; Atmospheric Chemical Compounds. Academic Press, Inc., Orlando, FL p. 93 (1986) (3) Austin S, Glowacki A; Hydrochloric acid In: Ullmann's Encyclopedia of Industrial Chemistry A13: 283-96 (1989) (4) Crummett WB; Chlorinated Dioxins and Related Compounds pp. 253-63 (1982) (5) Greim H; Chemosphere 20: 317-31 (1990) (6) Glasser H et al; J Air Waste Manage Assoc 41: 1180-8 (1991)]

Environmental Transport and Persistence:

Bioaccumulation: Not applicable. Based on the pK_a value of -6.1 (1), HCl in water will be fully dissociated to the chloride ion and therefore, would not be expected to bioconcentrate in aquatic organisms.

[(1) Dean JA; Langes Handbook of Chemistry 13th ed McGraw-Hill Book Co. p. 5-15 (1985)]

Volatilization/ Adsorption: The Henry's Law constant of 2×10^6 atm-m³/mole at 25°C (3) is based on the partial pressure of HCl over concentrated highly acidic aqueous solution (4). The pK_a value of -6.1 (1) indicates that HCl will dissociate to hydrogen ions and chloride ions at environmental pHs 5-9 and therefore, should not volatilize at the rate estimated from the Henry's Law constant. Since there are no Henry's Law constant

measurements available under environmental conditions, volatilization from water and environmental partitioning can not be estimated. In a field study of reclaimed water, the chloride ion has been shown to rapidly migrate when injected directly into an aquifer (2) which indicates low adsorption potential.

[(1) Dean JA; Langes Handbook of Chemistry 13th ed McGraw-Hill Book Co. p. 5-15 (1985) (2) Roberts PV et al; Water Res 16: 1025-35 (1982) (3) Betterton EA; Gas Pollut: Character Cycl; Nriagu JO Ed John Wiley & Sons, Inc. pp. 1-50 (1992) (4) Brimblecomb P, Clegg SL; J Atmos Chem 7: 1-18 (1988)]

Persistence: The pK_a value of -6.1 (1) indicates that HCl will dissociate to the chloride ion and the hydrogen ion at environmental pHs 5-9. Furthermore, the chloride ion is expected to be stable in the environment; it is a major constituent of natural waters with concentrations of 19,000 ppm in seawater, 0.2-17 mg/L in rain/snow samples, 2 mg/L in water from a reservoir, 13 mg/L in the Niagara River, and 9.6 ppm in well water from Dayton, OH (2).

[(1) Dean JA; Langes Handbook of Chemistry 13th ed McGraw-Hill Book Co. p. 5-15 (1985) (2) Snoeynik VL, Jenkins D; Water Chemistry. New York, NY: John Wiley & Sons pp. 3-14 (1980)]

Appendix A

United States Producers of HCl¹

Company Name	Location
Akzo Chemicals Inc.	Edison, NJ Gallipolis Ferry, WV
Allied-Signal Inc.	Baton Rouge, LA Danville, IL El Segundo, CA
Ausimont USA, Inc.	Thorofare, NJ
BASF Corp.	Geismar, LA
Borden Chemicals and Plastics Partnership	Geismar, LA
Cabot Corp.	Tuscola, IL
CIBA-GEIGY Corp.	McIntosh, AL St. Gabriel, LA
Degussa Corp.	Theodore, AL Waterford, NY
Detrex Corp.	Ashtabula, OH
Dover Chemical Corp.	Dover, OH
Dow Chemical U.S.A.	Freeport, TX Midland, MI Oyster Creek, TX Pittsburg, CA Plaquemine, LA La Porte, TX
Dow Corning Corp.	Carrollton, KY Midland, MI
Du Pont	Parkersburg, WV Antioch, CA Corpus Christi, TX Deepwater, NJ Louisville, KY Montague, MI La Place, LA

Company Name	Location
Elf Atochem North America, Inc.	Portland, OR Tacoma, WA Calvert City, KY Wichita, KS Riverview, MI
Ferro Corp.	Hammond, IN
FMC Corp.	Baltimore, MD Nitro, WV
Formosa Plastics Corp. U.S.A.	Baton Rouge, LA Point Comfort, TX
General Electric Co.	Mount Vernon, IN Waterford, NY
Georgia Gulf Corp.	Plaquemine, LA
The BFGoodrich Co.	La Porte, TX
Hanlin Group, Inc.	Acme, NC Brunswick, GA Orrington, ME
ICI Americas Inc.	Cold Creek, AL Geismar, LA Mount Pleasant, TN
ISK Biotech	Greens Bayou, TX
Jones-Hamilton Co.	Waldbridge, OH
La Roche Chemicals Inc.	Gramercy, LA
Magnesium Corp. of America	Rowley, UT
Magnetics International Inc.	Burns Harbor, IN
Miles Inc.	Baytown, TX New Martinsville, WV
Monsanto Co.	Bridgeport, NJ Sauget, IL
Occidental Chemical Corp.	Belle, WV Deer Park, TX Niagara Falls, NY Tacoma, WA

Company Name	Location
Olin Corp.	Augusta, GA Charleston, TN Lake Charles, LA
Oxymar	Ingleside, TX
Pioneer Chlor Alkali Co., Inc.	Henderson, NV
PPG Industries, Inc.	Barberton, Ohio Lake Charles, LA Natrium, WV La Porte, TX
Rhone-Poulenc Ag Co.	Institute, WV
Shell Chemical Co.	Norco, LA
Standard Chlorine Chemical Co., Inc.	Delaware City, DE
Velsicol Chemical Corp.	Chattanooga, TN Memphis, TN
Vista Chemical Co.	Baltimore, MD Lake Charles, LA
Vulcan Materials Co.	Geismar, LA Port Edwards, WI Wichita, KS
Westlake Monomers Corp.	Calvert City, KY
Weyerhaeuser Co.	Longview, WA
Witco Corp.	Phillipsburg, NJ

¹SRI International; 1993 Directory of Chemical Producers, United States of America pp. 678-81 (1993)

HYDROGEN FLUORIDE

SUBSTANCE IDENTIFICATION

Synonyms: Hydrofluoric acid; HF

Structure:



CAS Registry Number: 7664-39-3

Molecular Formula: HF

CHEMICAL AND PHYSICAL PROPERTIES

Boiling Point: 19.5°C

Melting Point: -83.37°C

Molecular Weight: 20.01

Dissociation Constants: $\text{pK}_a = 3.2$ (1)

Log Octanol/Water Partition Coefficient: Not available

Water Solubility: Infinite (4)

Vapor Pressure: 917 mm Hg @ 25 °C (2)

Henry's Law Constant: $1.04 \times 10^{-4} \text{ atm}\cdot\text{m}^3/\text{mole}$ @ 25 °C; under highly acidic conditions (3)

Lower Explosive Limit: Not available

[(1) Budavari S et al; The Merck Index. 11th ed Rahway, NJ: Merck & Co., Inc. pp. 758-9 (1989) (2) Daubert TE, Danner RP; Physical and Thermodynamic Properties of Pure Chemicals: Data Compilation Hemisphere Pub Corp New York, NY (1989) (3) Betterton EA; Gas Pollut: Character Cycl; Nriagu JO Ed John Wiley & Sons, Inc pp. 1-50 (1992) (4) Lide DR; CRC Handbook of Chemistry and Physics 71st ed Boca Raton, FL: CRC Press, Inc. p. 4-67 (1990)]

EXPOSURE PROFILE

Production: In 1991, 161,000 tons (322 million pounds) of hydrogen fluoride were produced in the U.S.; an additional 114,000 tons (228 million pounds) were imported, primarily from Mexico and Canada (1). Exports are negligible (1). Hydrogen fluoride is produced by Allied-Signal (Geismar, LA), Du Pont (La Porte, TX), and Atochem North America (Calvert City, KY) (1).

[(1) Chemical Marketing Reporter; Chemical Profile: Hydrofluoric acid. July 29, 1991]

Use: Hydrogen fluoride is primarily used in the production of fluorocarbons (58%). It is also used in aluminum manufacture (captive HF) (15%), petroleum alkylation catalysis (4%), stainless steel pickling (4%), aluminum manufacture (merchant HF) (3%), and miscellaneous uses,

including glass etching, herbicide manufacture, rare metals, fluoride salts, and specialty fluorides (13%) (1). The hydrogen fluoride consumed by the aluminum industry (18% of production) is used to produce synthetic cryolite, which is used in the reduction of aluminum in electrolysis cells; this process gives off hydrogen fluoride which may be recycled (captive HF) (4, 5). Hydrogen fluoride is also used in the production of branched alkane motor fuels, aerosols, plastics, and refrigerants (2). In the field of atomic energy, it is used in the production of uranium tetrafluoride from uranium oxide, and it is used in certain types of rocket fuels (2). Hydrogen fluoride is also used in cleaning cast iron, copper, and brass; removing efflorescence from brick and stone, or sand particles from metallic castings; working over too heavily weighted silks; frosting and etching glass and enamel; polishing crystal glass; decomposing cellulose; enameling and galvanizing iron; and increasing porosity of ceramics (3). Hydrogen fluoride salts are used as insecticides, to arrest undesirable fermentation in brewing, and in analytical work to determine SiO_2 (3).

[(1) Chemical Marketing Reporter; Chemical Profile: Hydrofluoric acid. July 29, 1991 (2) Waldbott GL, Lee JR; Clinical Toxicology 13: 391-402 (1978) (3) Budavari S et al; The Merck Index. 11th ed Rahway, NJ: Merck & Co., Inc. pp. 758-9 (1989) (4) Anderson WA, Haupin WE; Aluminum and Alloys. In: Kirk-Othmer Encyclopedia of Chemical Technology John Wiley & Sons 2: 129-188 (1978) (5) Jaccaud M, Faron R; Fluorine Ullmann's Encyclopedia of Industrial Chemistry A11: 294 (1988)]

Occupational Exposure: NIOSH (NOES Survey 1981-83) has statistically estimated that 182,589 workers are exposed to hydrogen fluoride in the United States (1). Hydrogen fluoride concentrations ranged from 0.34 to 3 mg/m^3 in the air of the etching department at the Eagle Convex Glass Company in Clarksburg, WV (2). The highest concentration of hydrogen fluoride normally found in the atmosphere of a nuclear submarine was 0.3 ppm (3). In Poland, a worker in an electrolysis shop of an aluminum plant had been exposed to fluoride compounds; tests of the hydrogen fluoride concentration at his work station in 1980 showed a concentration of 6-22 times greater than permissible (permissible exposure limit not defined) (4). Workers in the finishing room of a polytetrafluoroethylene (PTFE) plant were exposed to hydrogen fluoride in the atmosphere immediately outside the oven where PTFE is heated above normal drying temperatures; data were not quantified (5). From 1961 to 1971, estimated hydrogen fluoride atmospheric concentrations surrounding an alkylation unit at a major oil company were over 25 ppm during acid tank gauging, 25-200 ppm during shutdown for repair, and 3 ppm during every day duty (6). On September 15 and 16, 1981, workplace air concentrations of hydrogen fluoride were 2.0 and 1.1 mg/m^3 , respectively, around the acid line of a hard chrome plating production shop (7). Qualitative detections suggest that workers in superphosphate, enamel, and fertilizer factories, and welders, garage workers, and waterworks employees may be exposed to hydrogen fluoride (8).

[(1) NIOSH. National Institute for Occupational Safety and Health. National Occupational Exposure Survey (NOES). Computer printout March 29, 1989 (2) Baron S et al; Health Hazard Evaluation Report No. HETA-89-137-2005 Eagle Convex Glass Company, Clarksburg, WV NIOSH U.S. Department of Health and Human Services, Cincinnati, OH (1990) (3) Schaefer KE; Atmospheric Requirements of Confined Spaces 9: 320-31 (1964) (4) Miszke A et al; Nasal septum and Mucosa in fluorosis; Department of Laryngology and Cytological and Microscope Laboratories, Narutowicz Hospital, Cracow, Poland 17: 114-8 (1984) (5) Adams WGF; Trans Ass Industr Med Offrs 13: 20-1 (1963) (6) Waldbott GL, Lee JR; Clinical Toxicology 13: 391-402 (1978) (7) Sheehy JW; In-depth survey report of U.S. Chrome Fond Du Lac,

Wisconsin: National Institute for Occupational Safety and Health, Cincinnati, OH (1982) (8) The Committee on Toxicology, National Academy of Sciences Washington DC Report No. APTD-0765 NTIS PB203-465 (1971)]

Consumer Exposure: No data are available that suggest there is any consumer exposure to hydrogen fluoride.

Environmental Release and General Population Exposure: According to the 1991 Toxics Release Inventory (TRI), 9.2 million pounds of hydrogen fluoride were released to the environment, of which 99.7% was released into the atmosphere (1).

Hydrogen fluoride may be released to the atmosphere in emissions during its production and from manufacturing aluminum, brick, glass, pottery, ceramics, electronics, fertilizers, lacquers, fluorocarbons, phosphoric acid, and steel (2, 4). It may also be released to the atmosphere in emissions from petroleum refining, ferroenamel production, welding processes, foundries and metal fabricating plants, coal combustion, rockets, and volcanoes (2, 4). Coal may contain 40-295 ppm fluoride depending on its source, some of which is released as hydrogen fluoride during combustion (4). Air concentrations of hydrogen fluoride ranged from 0.2 to 0.3 mg/m³ in emissions from a modern German municipal waste incinerator (3).

Based on the above data, residents downwind from effluent stacks may be exposed to hydrogen fluoride in air (4). People living in homes or areas where homes are heated with coal may be exposed to hydrogen fluoride in air.

Hydrogen fluoride is an atmospheric transformation product of formylfluoride (HC(O)F) which is the major atmospheric oxidation product of hydrofluorocarbons HFC-134a and HFC-41 (5). Therefore, concentrations of hydrogen fluoride are expected to be low (in the parts per billion range) in rainwater as a result of the release of HFCs (5).

[(1) U.S. EPA; Toxics Release Inventory (1992) (2) Graedel TE et al; Atmospheric Chemical Compounds Orlando, FL: Academic Press, Inc. p. 93 (1986) (3) Greim H; Chemosphere 20: 317-31 (1990) (4) The Committee on Toxicology, National Academy of Sciences Washington DC Report No. APTD-0765 NTIS PB203-465 (1971) (5) Wallington TJ; Environ Sci Technol 27: 1448-52 (1993)]

Environmental Transport and Persistence:

Bioaccumulation: Based on hydrogen fluoride's miscibility in water (1) and pK_a of 3.2 (2), hydrogen fluoride in water will be dissociated to the fluoride ion and hydrogen ion and would not be expected to bioconcentrate in aquatic organisms.

[(1) Lide DR; CRC Handbook of Chemistry and Physics 71st ed Boca Raton, FL: CRC Press, Inc. p. 4-67 (1990) (2) Budavari S et al; The Merck Index. 11th ed Rahway, NJ: Merck & Co., Inc. pp. 758-9 (1989)]

Volatilization/ Adsorption: The Henry's Law constant of 1.04×10^{-4} atm-m³/mole at 25 °C (1) is based on the partial pressure of hydrogen fluoride over concentrated highly acidic aqueous solution (3). Based on a pK_a of 3.2 (2), hydrogen fluoride will be

approximately 99% dissociated at environmental pHs of 5-9 and therefore, may not volatilize at the rate estimated from the Henry's Law constant. Since there are no data available under environmental conditions, volatilization from water and environmental partitioning can not be estimated. No data are available indicating that the fluoride ion adsorbs to sediments and soil.

[(1) Betterton EA; Gas Pollut: Character Cycl; Nriagu JO Ed John Wiley & Sons, Inc pp.1-50 (1992) (2) Budavari S et al; The Merck Index. 11th ed Rahway, NJ: Merck & Co., Inc. pp. 758-9 (1989) (3) Brimblecomb P, Clegg SL; J Atmos Chem 7: 1-18 (1988)]

Persistence: The pK_a value of 3.2 (1) indicates that hydrogen fluoride will dissociate to the fluoride ion and the hydrogen ion at environmental pHs (5-9). Furthermore, the fluoride ion is expected to be stable in the environment; natural soft waters and seawater contain about 0.2 mg/L and 1-1.4 mg/L fluoride ion, respectively (2).

[(1) Budavari S et al; The Merck Index. 11th ed Rahway, NJ: Merck & Co., Inc. pp. 758-9 (1989) (2) Jaccaud M, Faron R; Fluorine Ullmann's Encyclopedia of Industrial Chemistry A11: 294, 323 (1988)]

CHLORINE

SUBSTANCE IDENTIFICATION

Synonyms: Molecular chlorine; bertholite

Structure:



CAS Registry Number: 7782-50-5

Molecular Formula: Cl_2

CHEMICAL AND PHYSICAL PROPERTIES

Boiling Point: -34.6°C

Melting Point: -100.98°C

Molecular Weight: 70.9

Dissociation Constants: Not available

Log Octanol/Water Partition Coefficient (Log K_{ow}): Not available

Water Solubility: 6,400 mg/L @ 25°C (1)

Vapor Pressure: 5,854 mm Hg @ 25°C (2)

Henry's Law Constant: $8.53 \times 10^{-2} \text{ atm}\cdot\text{m}^3/\text{mole}$ @ 25°C (estimated from vapor pressure and water solubility) (3)

Lower Explosive Limit: Not available

[(1) Cotton FA, Wilkinson G; Advanced Inorganic Chemistry 2nd ed New York, NY: Interscience Publishers John Wiley & Sons p. 569 (1966) (2) Daubert TE, Danner RP; Physical and Thermodynamic Properties of Pure Chemicals: Data Compilation New York, NY: Hemisphere Pub Corp (1989) (3) Lyman et al; Handbook of Chemical Property Estimation Methods, Washington DC: American Chemical Society Chapter 15 (1990)]

EXPOSURE PROFILE

Production: In 1992, 22.28 billion pounds of chlorine were produced in the United States (1). U.S. producers of chlorine are tabulated in Appendix A.

[(1) Reisch MS; Chem Eng News pp. 10-13 and 16 April 12 (1993)]

Use: The manufacture of vinyl chloride monomer (27%) is the largest chlorine use (1). Chlorine is also used to bleach pulp and paper (14%), in the production of polyurethanes (14%), solvents (13%), other organics (12%), inorganics (9%), titanium dioxide (6%), and in water treatment (5%) (1). Chlorine is used in the production of propylene oxide, carbon tetrachloride, perchloroethylene, hypochlorite, epichlorohydrin, 1,1,1-trichloroethane, methylene chloride,

ethylene dichloride (solvent and trade), trichloroethylene, chlorobenzene, chloroprene, bromine, and several other organic and inorganic compounds (2). Chlorine is a slimicide and it is used as a sanitizing and disinfecting agent for municipal water supplies and swimming pools (2). Chlorine is also used as an etching gas in the semiconductor industry (3). Chlorine is used in sewage treatment and in the pharmaceutical and textile industries (4).

[(1) Chemical Marketing Reporter; Chemical Profile: Chlorine. June 1, 1992 (2) Curlin LC et al; Kirk-Othmer Encyclopedia of Chemical Technology 4th ed John Wiley & Sons 1: 938-1025 (1991) (3) Sherin BJ; Risk Assessment and Control of Toxic Gas Releases Hazard Assessment and Control Technology in Semiconductor Manufacturing, Chelsea, MI: Lewis Pub, Inc. pp. 115-33 (1989) (4) Broderick A, Schwartz DA; Hazardous Materials Toxicology, Clinical Principles of Environmental Health, JB Sullivan, Jr, GR Krieger Eds, Baltimore, MD: Williams and Wilkins pp. 791-6 (1992)]

Occupational Exposure: NIOSH (NOES Survey 1981-83) has statistically estimated that 170,000 workers are exposed to chlorine in the United States (1). Workers were exposed to high levels of chlorine gas in the cell rooms of a chlor-alkali facility (2). At water treatment facilities, the chlorination process poses hazards of escaping chlorine and potential worker exposure (3). During a respiratory health survey conducted in 1988, 78 of 316 pulpmill workers had at least one chlorine exposure incident in their work histories (4). High concentrations of chlorine were detected in generator buildings of pulp and paper industries, particularly during start ups, shut downs, and following collection of quality control samples (6). Chlorine concentrations ranged from 0.09 to 1.59 ppm in workplace air from four sites in a pulp bleaching facility (12). Chlorine concentration ranges were 0.14 to 0.2, 0.14 to 0.18, and 0.1 to 0.16 ppm in air samples taken at a pulp bleaching factory using different test methods (13). Accidental chlorine gas exposures were around or below 1 ppm in a British Columbia pulpmill; however, exposures as high as 15 ppm were measured in the pulping department (14). Furthermore, a total of 189 workers at this pulpmill reported one or more exposure incidents in the past (14). During the production of strontium, workers are potentially exposed to chlorine (5). Free chlorine has been identified in the air of indoor swimming pools during periods of high pool crowding and poor ventilation (7); therefore, lifeguards and other pool workers may be exposed to chlorine in the atmospheres of indoor swimming pools. In the semiconductor industry, workers are potentially exposed to chlorine gas when it is used during the etching process (8). Concentrations of chlorine gas in area air samples were less than 0.2 ppm in the central supply area of a hospital where an overloaded exhaust system existed (9). Four septic tank workers were exposed to high levels of chlorine gas while cleaning out a wastewater tank at a chicken hatchery (10). Worker exposure to chlorine has been identified during the production of epichlorohydrin (11).

[(1) NIOSH. National Institute for Occupational Safety and Health. National Occupational Exposure Survey (NOES). Computer printout March 29, 1989 (2) Reh CM et al; Hazard Evaluation Report No. HETA-87-402-2145 LCP Chemicals and Plastics, Inc., Brunswick, GA NIOSH U.S. Department of Health and Human Services, Cincinnati, OH (1991) (3) McCunney RJ; Am J Ind Med 9: 271-9 (1986) (4) Salisbury DA et al; Am J Ind Med 20: 71-81 (1991) (5) Saric M; Encyclopedia of Occupational Health and Safety 2: 2111-2 (1983) (6) Schoultz K et al; Control technology assessment in the pulp and paper industry NIOSH U.S. Department of Health and Human Services, Cincinnati, OH (1983) (7) Shaw JW; Proceedings of the American Society of Heating, Refrigerating and Air-Conditioning Engineers, Inc. Conference April 20-23 Atlanta, GA pp. 83-7 (1986) (8) Sherin BJ; Risk Assessment and Control of Toxic Gas Releases Hazard Assessment and Control Technology in Semiconductor Manufacturing, Chelsea, MI: Lewis Pub, Inc. pp. 115-33 (1989) (9) Zey JN et

al; Hazard Evaluation Report No. HETA-85-292-1811 Clark County Hospital, Jeffersonville, IN NIOSH U.S. Department of Health and Human Services, Cincinnati, OH (1987) (10) NIOSH; Division of Safety Research, NIOSH, U.S. Department of Health and Human Services, Morgantown, WV Report No. FACE-86-38 (1986) (11) Barbone F et al; Am J Ind Med 22: 835-49 (1992) (12) Bjorkholm E et al; J Chromato 457: 409-14 (1988) (13) Bjorkholm E et al; Appl Occup Environ Hyg 5: 767-70 (1990) (14) Kennedy SM et al; Am Rev Resp Dis 143: 74-9 (1991)]

Consumer Exposure Chlorine is in equilibrium with sodium hypochlorite (liquid bleach) in solution (2). Commercial strength liquid bleach used in swimming pools contains 12-15% chlorine and household bleach contains about 5% chlorine (3). Therefore, during its use as a sanitizing and disinfecting agent (1), people who use or maintain swimming pools may be exposed to chlorine and anyone using liquid bleach in the home may be exposed to chlorine.

[(1) Curlin LC et al; Kirk-Othmer Encyclopedia of Chemical Technology 4th ed New York, NY: John Wiley & Sons 1: 938-1025 (1991) (2) Farr JP et al; Kirk-Othmer Encyclopedia of Chemical Technology 4th ed New York, NY: John Wiley & Sons 4: 271-300 (1992) (3) Wojtowicz JA; Kirk-Othmer Encyclopedia of Chemical Technology 4th ed New York, NY: John Wiley & Sons 5: 932-968 (1993)]

Environmental Release and General Population Exposure: According to the 1991 Toxics Release Inventory (TRI), 78.498 million pounds of chlorine were released to the environment, of which 98.9% was released into the atmosphere (1).

Chlorine gas emissions averaged 100.5 mg/m³ with a standard deviation of 72 mg/m³ from a waste incinerator at a U.S. Army hospital; the variability in the plastic content of the waste, about 30%, accounts for the large standard deviation in the concentration of chlorine (2). Chlorine may also be released to the atmosphere in emissions from aluminum manufacturing, HCl manufacturing, refuse combustion, sewage treatment, wood pulping, and titanium and zinc manufacturing (5).

Free chlorine has been identified in the atmospheres of indoor swimming pools during periods of high pool crowding and poor ventilation (3); therefore, the general population may be exposed to chlorine in the air of indoor swimming pools.

The general population may be exposed to chlorine gas in the air following accidental discharges or spills; several people were exposed to chlorine after a spill in a railroad accident on February 26, 1978, in Youngstown, FL (4).

Free chlorine occurs naturally in volcanic gases (6).

[(1) U.S. EPA; Toxics Release Inventory (1992) (2) Murnyak GR, Guzewich DC; J Environ Health 45: 83-5 (1982) (3) Shaw JW; Proceedings of the American Society of Heating, Refrigerating and Air-Conditioning Engineers, Inc. Conference April 20-23 Atlanta, GA pp. 83-7 (1986) (4) Jones RN et al; Am Rev Resp Dis 134: 1190-5 (1986) (5) Graedel TE et al; Atmospheric Chemical Compounds Orlando, FL: Academic Press, Inc. p. 93 (1986) (6) Schmittinger P et al; Ullmann's Encyclopedia of Industrial Chemistry A6: 399-481 (1986)]

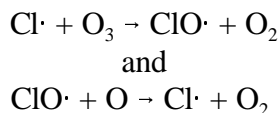
Environmental Transport and Persistence:

Bioaccumulation: Not applicable.

Volatilization/ Adsorption: Based on a measured water solubility of 6,400 mg/L at 25°C (1) and a measured vapor pressure of 5,854 mm Hg at 25°C (2), the Henry's Law constant for chlorine can be estimated to be 8.53×10^{-2} atm-m³/mole at 25 °C (3). According to a suggested classification scheme (3), volatilization from water with low organic content should be rapid. Chlorine is a strong oxidizing agent and the hypochlorous acid (HOCl⁺), which is contained in aqueous solutions of chlorine (1), should react with organic matter available in water or soil (4).

[(1) Cotton FA, Wilkinson G; Advanced Inorganic Chemistry 2nd Ed Interscience Publishers John Wiley & Sons New York, NY p. 569 (1966) (2) Daubert TE, Danner RP; Physical and Thermodynamic Properties of Pure Chemicals: Data Compilation New York, NY: Hemisphere Pub Corp (1989) (3) Lyman RJ et al; Handbook of Chemical Property Estimation Methods, Washington, DC: American Chemical Society Chapter 15 (1990) (4) Schmittinger P et al; Ullmann's Encyclopedia of Industrial Chemistry A6: 399-481 (1986)]

Persistence: In the environment, chlorine (Cl₂) is not expected to persist for long periods of time; it is a strong oxidizing agent with many end products (1). The number of possible reactions and therefore, the number of intermediates and products are very large, especially in water (1). For example, chlorine reacts with water to form hypochlorites and with organic compounds (1). Chlorine reacts vigorously with ammonia (1). Wet chlorine attacks most metals to form chlorides (1). Chlorine is also expected to have a short atmospheric lifetime (2). Because it is photosensitive, chlorine will dissociate to chlorine radicals, which will react with virtually any organic molecule (2). In the stratosphere, chlorine radicals are involved in a catalytic cycle with ozone and oxygen atoms shown below (2).



[(1) Schmittinger P et al; Ullmann's Encyclopedia of Industrial Chemistry A6: 399-481 (1986) (2) Graedel TE et al; Atmospheric Chemical Compounds Orlando, FL: Academic Press, Inc. pp. 70-71 (1986)]

Appendix A

United States Producers of Chlorine¹

Company Name	Location
Ashta Chemicals, Inc.	Ashtabula, OH
Cedar Chemical Corp.	Vicksburg, MS
Dow Chemical U.S.A.	Freeport, TX Plaquemine, LA
Du Pont	Niagara Falls, NY
Elf Atochem North America, Inc.	Portland, OR Tacoma, WA
Formosa Plastics Corp. U.S.A.	Baton Rouge, LA
Fort Howard Corp.	Green Bay, WI Muskogee, OK Rincon, GA
General Electric Co.	Burkville, AL Mount Vernon, IN
Georgia Gulf Corp.	Plaquemine, LA
Georgia-Pacific Corp.	Bellingham, WA Brunswick, GA
The BFGoodrich Co.	Calvert City, KY
Hanlin Group, Inc.	Acme, NC Brunswick, GA Orrington, ME
La Roche Chemicals Inc.	Gramercy, LA
Magnesium Corp. of America	Rowley, UT
Miles Inc.	Baytown, TX
Niachlor Inc.	Niagara Falls, NY

Company Name	Location
Occidental Chemical Corp.	Convent, LA Corpus Christi, TX Deer Park, TX Delaware City, DE La Porte, TX Mobile, AL Muscle Shoals, AL Niagara Falls, NY Tacoma, WA Taft, LA
Olin Corp.	Augusta, GA Charleston, TN McIntosh, AL
Oregon Metallurgical Corp.	Albany, OR
Pioneer Chlor Alkali Co., Inc.	Henderson, NV St. Gabriel, LA
PPG Industries, Inc.	Lake Charles, LA Natrium, WV
Titanium Metals Corp.	Henderson, NV
Vulcan Materials Co.	Geismar, LA Port Edwards, WI Wichita, KS
Weyerhaeuser Co.	Longview, WA

¹SRI International; 1993 Directory of Chemical Producers, United States of America pp. 517-518 (1993)